



HELIOS

Berkeley Lab Energy Research Strategy

Demand



Energy Efficiency

Energy Policy

Supply



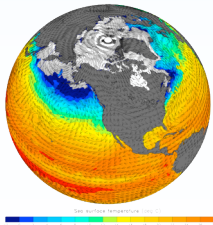
Bioenergy

Geological
Approaches

Materials &
Non-living
Systems

Nuclear

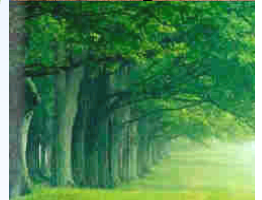
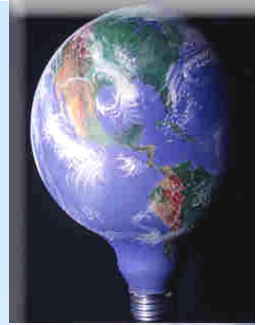
Consequences



Climate
Change

Carbon
Sequestration

Water
Resources



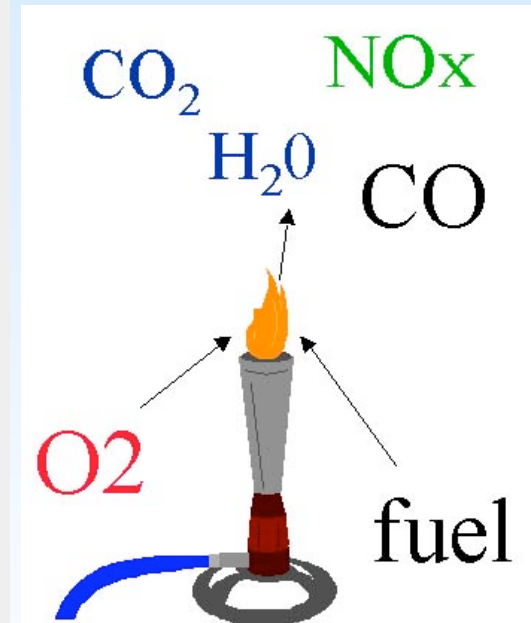
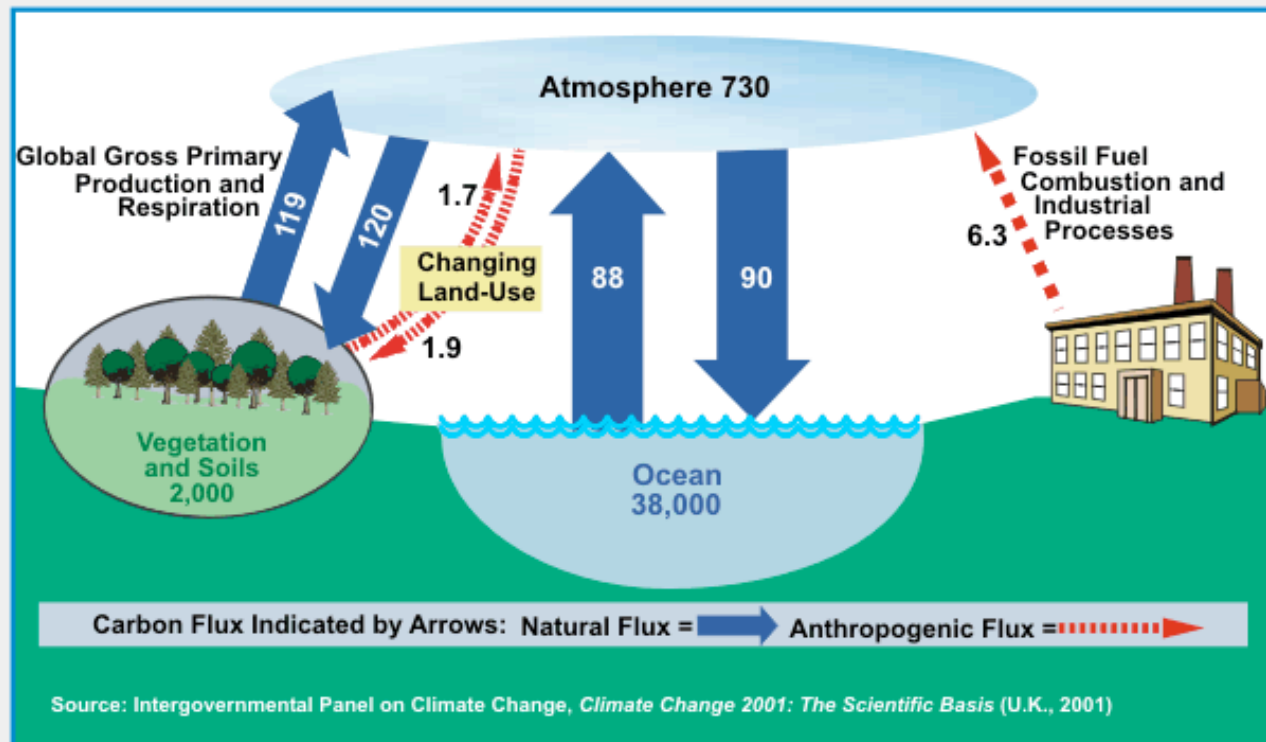


HELIOS

Remember all those Cycles you learned about?



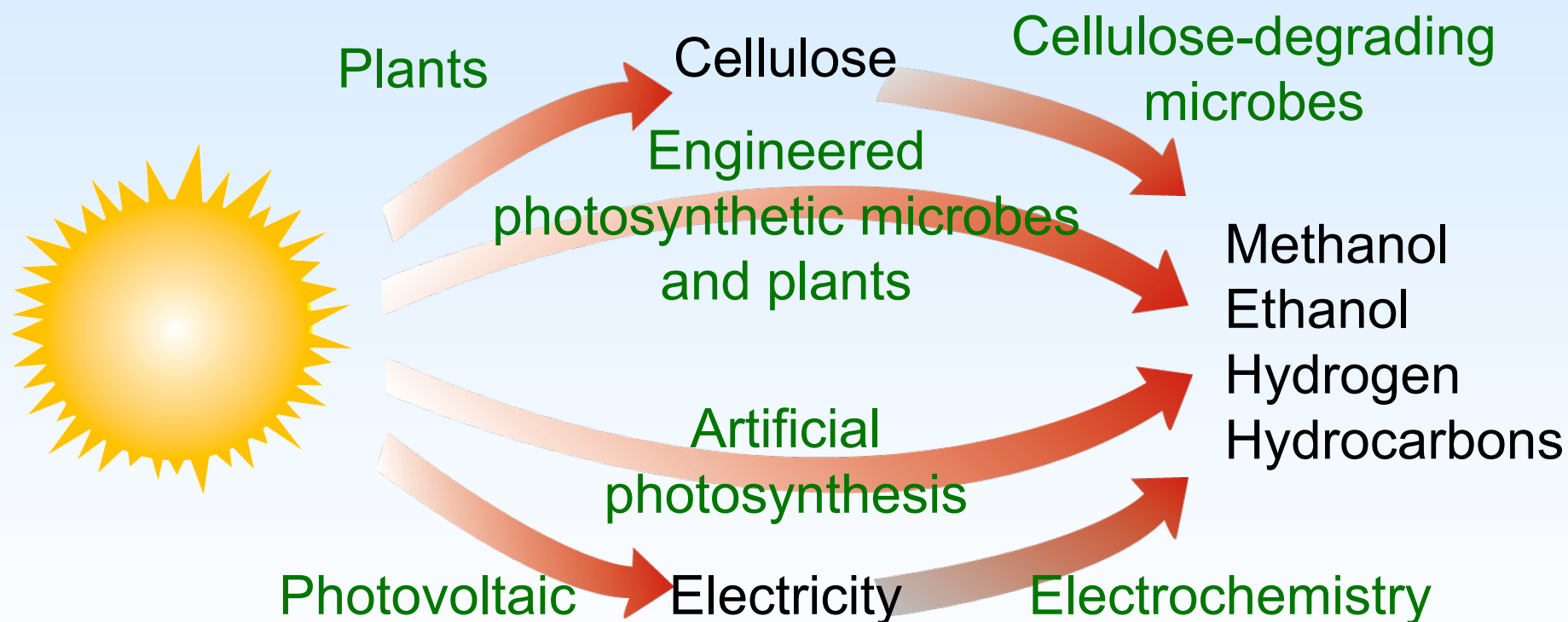
They matter, because half a cycle on a global scale is not sustainable



The ocean and vegetation are able to absorb only 3.2 of mankind's annual 6.3 billion metric tons of excess carbon emissions, leaving 3.1 billion metric tons more in the atmosphere each year



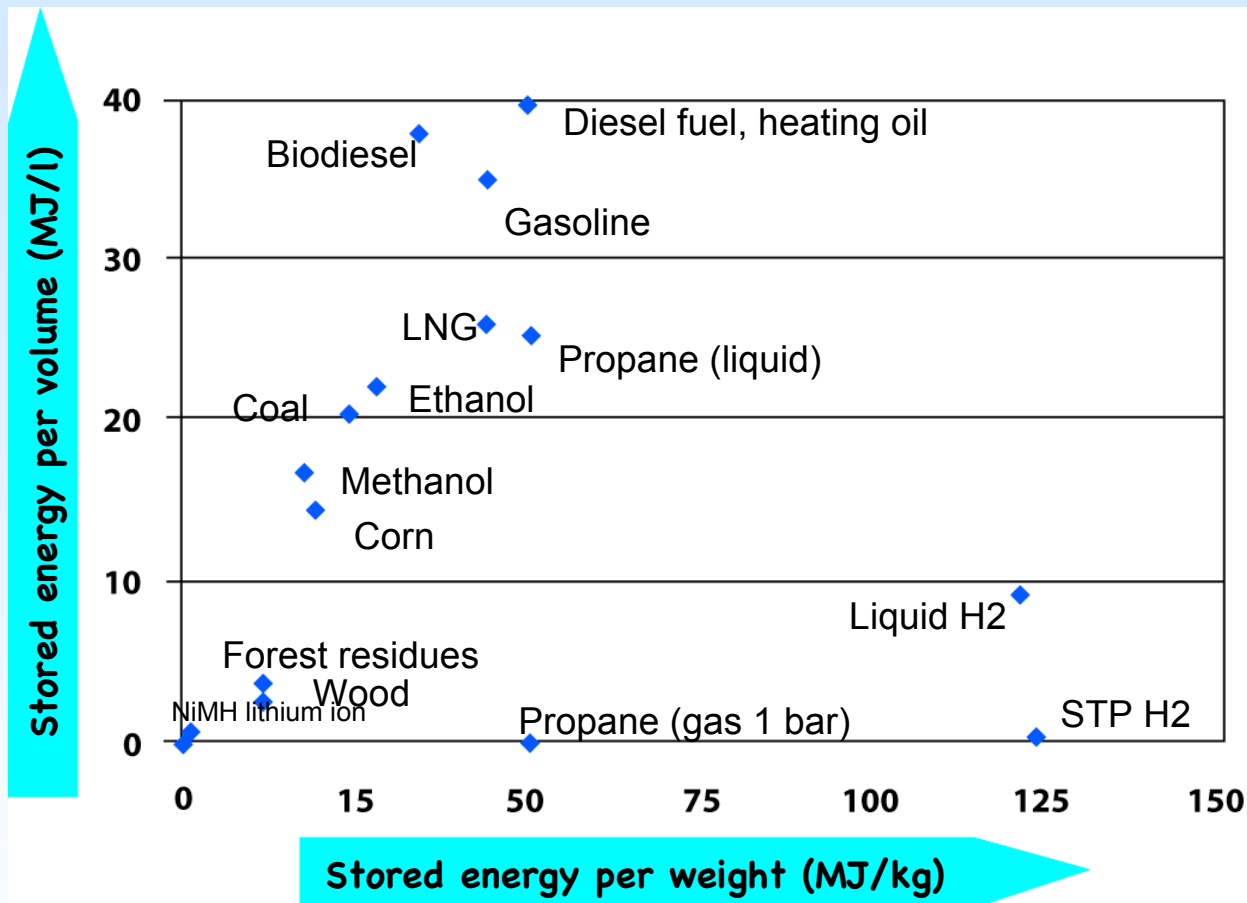
Helios Program in Solar Fuels Generation: complete the combustion cycle





HELIOS

Why liquid fuels?



High energy per volume,
“transportable”

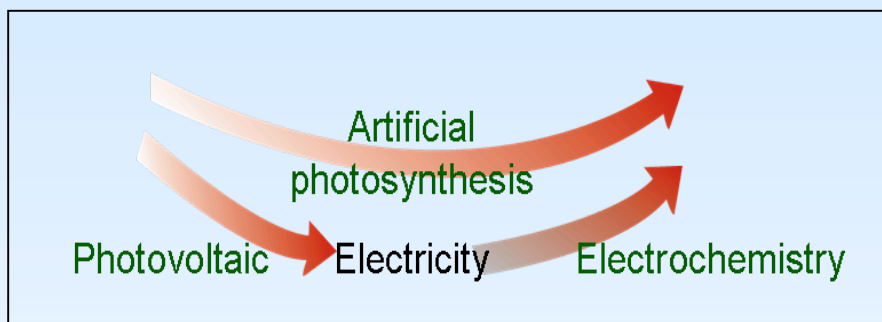
Examples: 10 gallons of gasoline vs. battery

(assumptions: *internal combustion engine*: 38% eff , 17% losses from idling; NiMH battery: .36MJ/l, 60% extractable; Li-Ion Battery: .9 MJ/l, 95% extractable; *electric engine*: 90% eff)

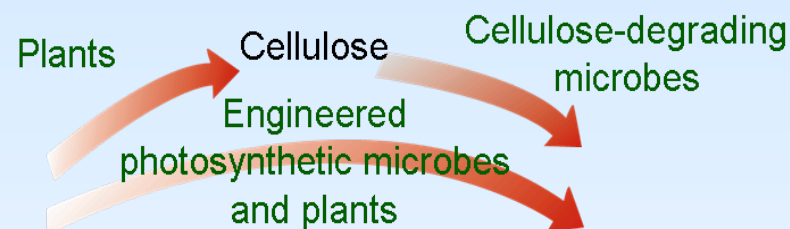
273,3 MJ deliverable	Gasoline, 10 gallons	NiMH	Li Ion
volume	1.3 cu ft	29.8 cu ft	12.5 cu ft
weight	61.6 lb (+250-750 lb eng)	5,060 lb	1,172 lb



Major Helios Approaches to Solar Derived Fuels



Helios Nanomaterials



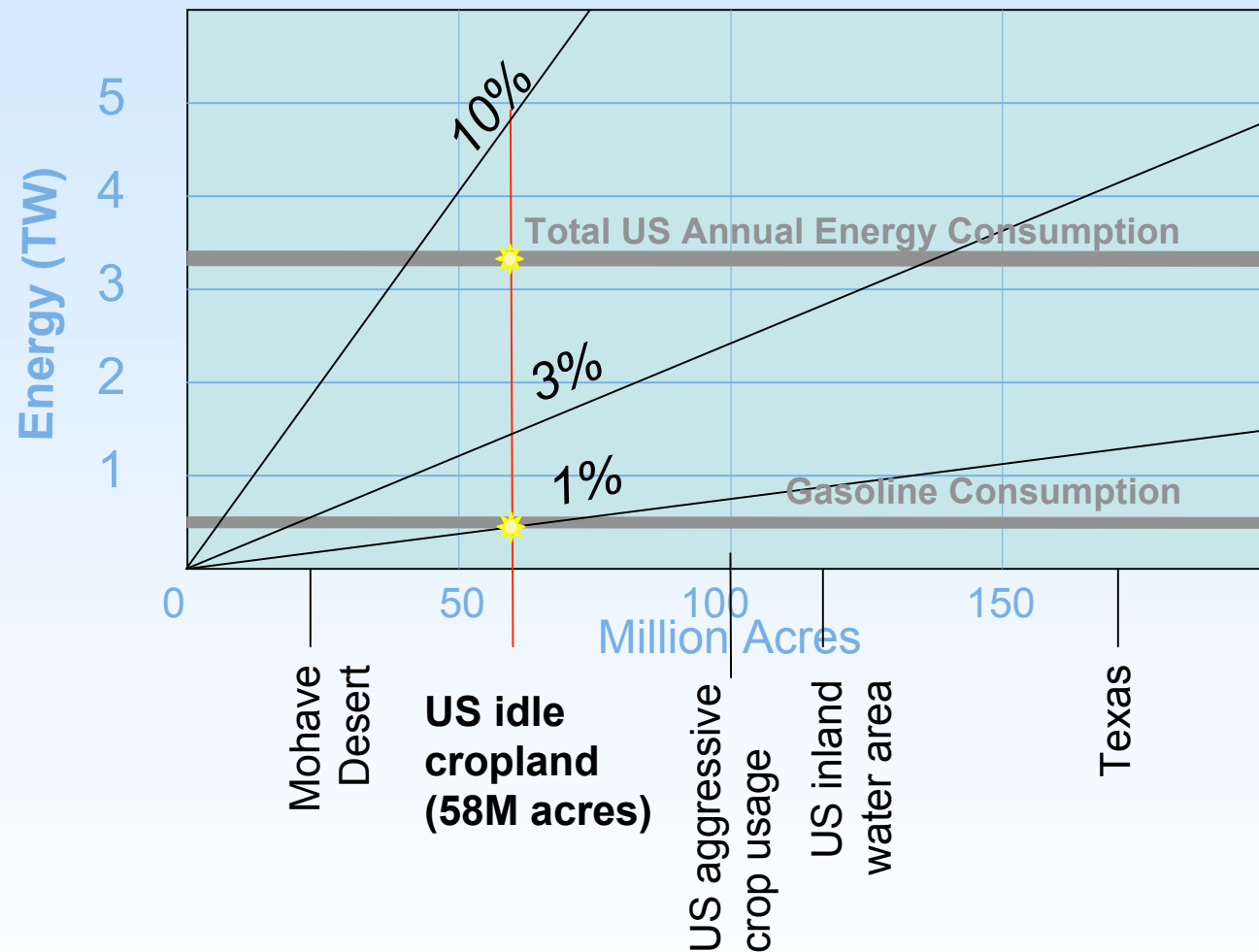
Helios Biofuels

- Scale of the solar fuel problem
- Efficiency needed
- How nanomaterials can contribute to a new solution



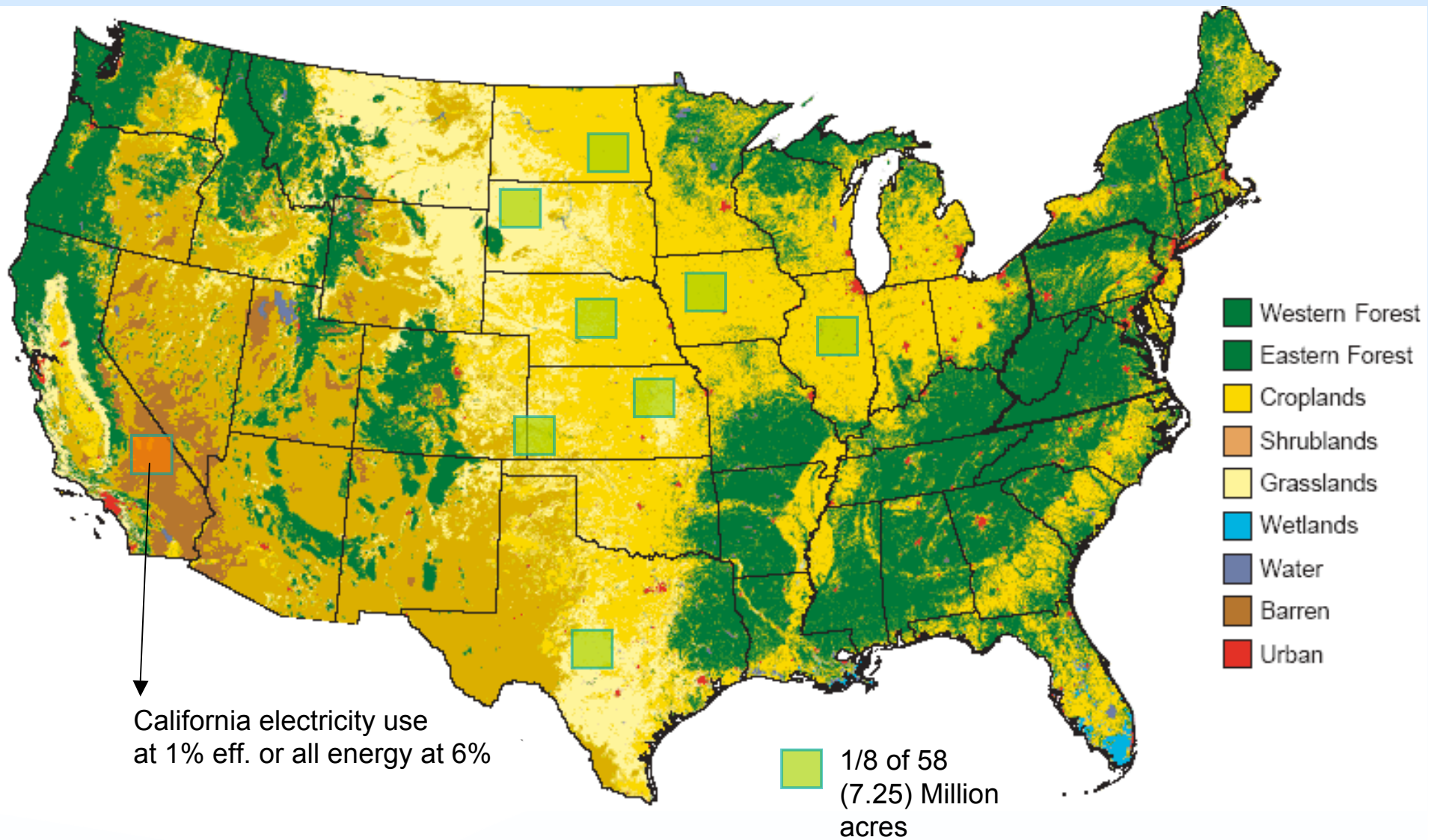
HELIOS

Solar efficiency and land usage



Our goal: Demonstrate within ten years a solar fuel generator that uses abundant materials and scalable manufacturing processes, that has an overall stable power efficiency of $> 1\%$ from sunlight, and that yields a chemically pure fuel having an energy density at least as large as that of methanol (4,600Wh/l, 6,400Wh/kg)

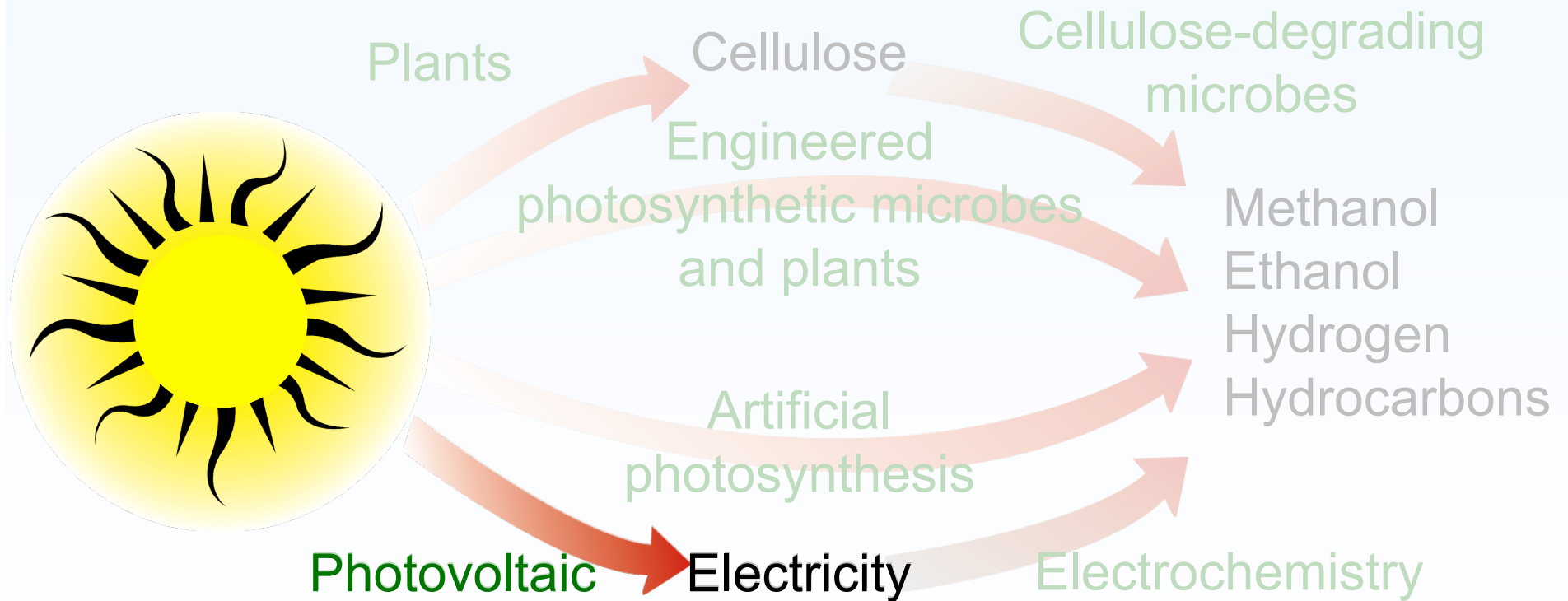
58M acres – how big is that?





HELIOS

Helios PV: Sunlight to Electricity

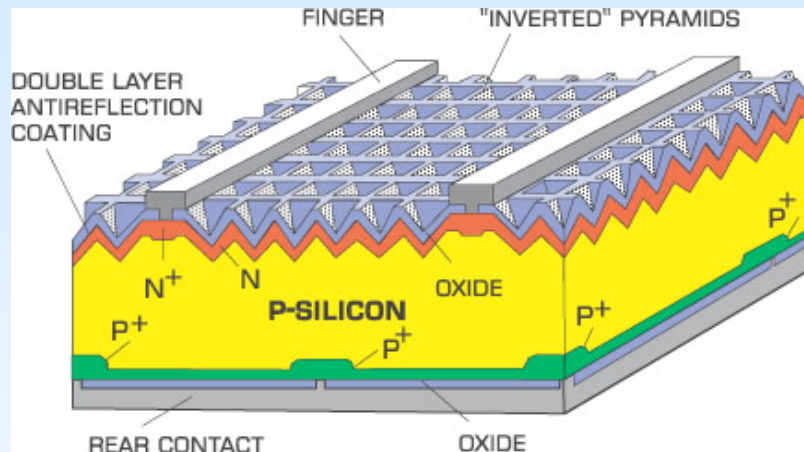




HELIOS



Solar cells based on
inorganic single crystals *are* well-established...



Si ~22-24%
Power efficiency
Photon to electricity

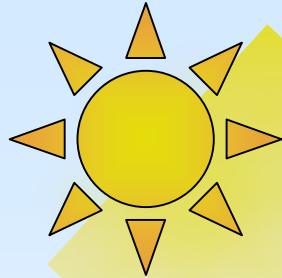
...but new phenomena on the nanoscale, coupled with the possibility of new fabrication methods, suggest taking a closer look at nanoscale PVs



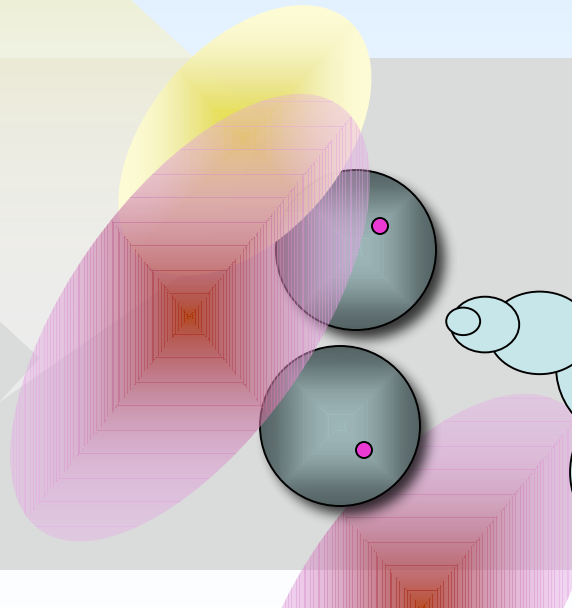
HELIOS



How a solar cell works:
An incident packet of solar energy—a photon—kicks an electron out of an atom, if it has enough energy



One electron off in the conduction band, now!



The electrons are still bound to these atoms!

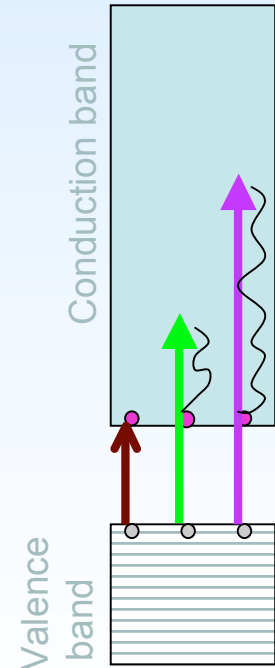
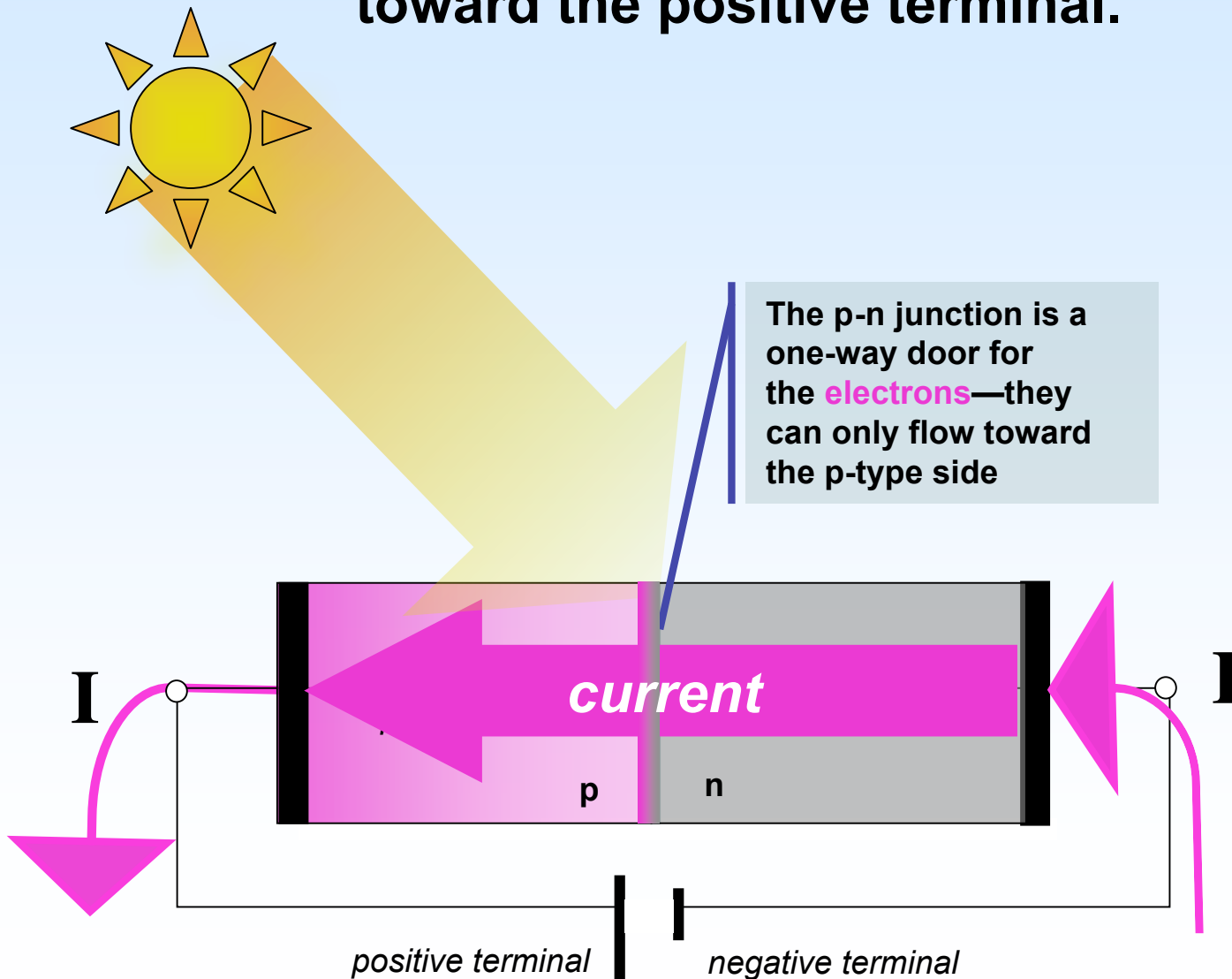
It takes a certain amount of energy to break an electron loose from its “bound” state in a semiconductor—the “energy gap”.



HELIOS



A silicon solar cell absorbs sunlight. Light quanta boost **electrons** into the conduction band and produce **electric current** that flows toward the positive terminal.



The efficiency of a semiconductor PV is related to its energy gap —Silicon is almost ideal

Small energy gap, much
energy absorbed is
transformed to heat

31%*

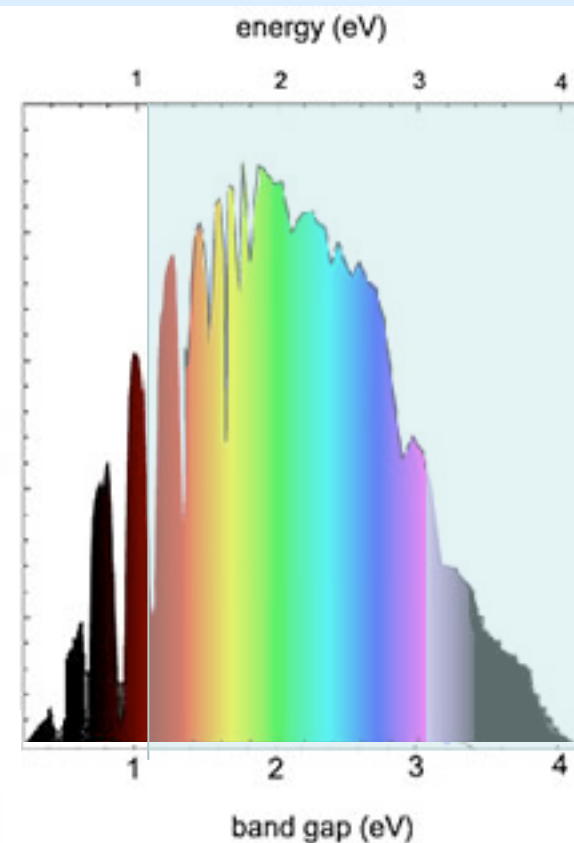
Efficiency

1.1 eV

Gap energy

Large energy gap, not
able to absorb
enough
energy from
sunlight

solar flux
(photons per
unit area per
unit time)

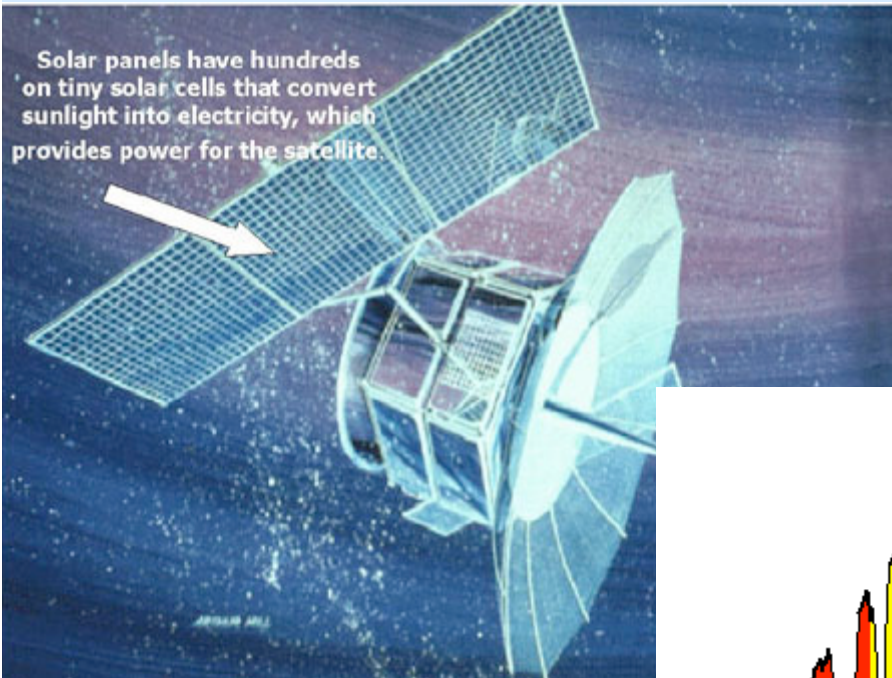


*ultimate efficiency, room
temp-- idealized model

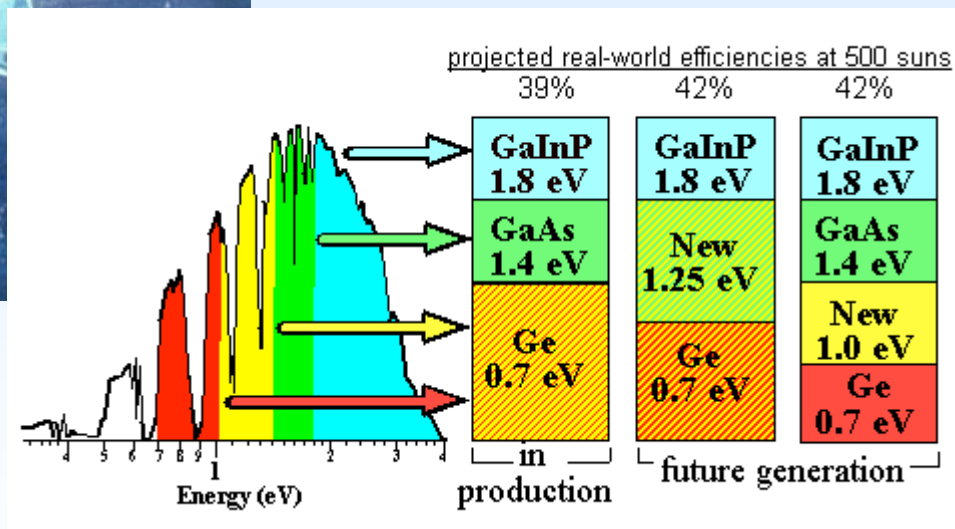


HELIOS

Satellite Solar Cells



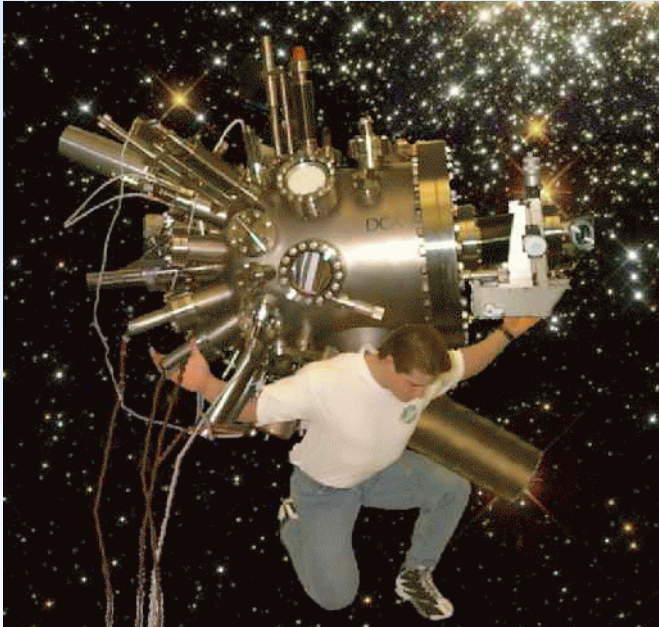
**III-V multi-gap
~35-40%, 50%?**



Is it possible to make a huge area
of very efficient solar cells?



Issues of scale of production vs. efficiency of device



Very efficient, but not scalable

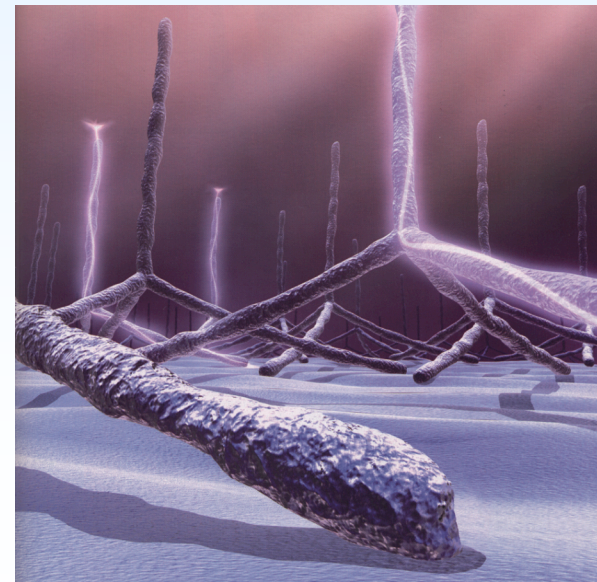
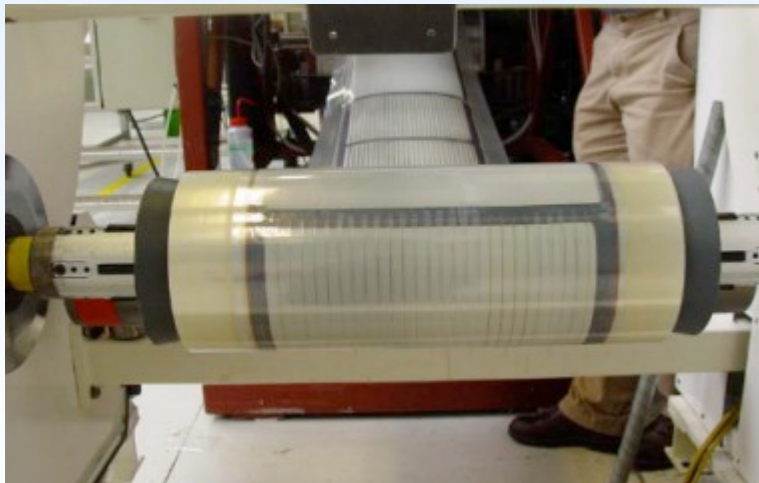
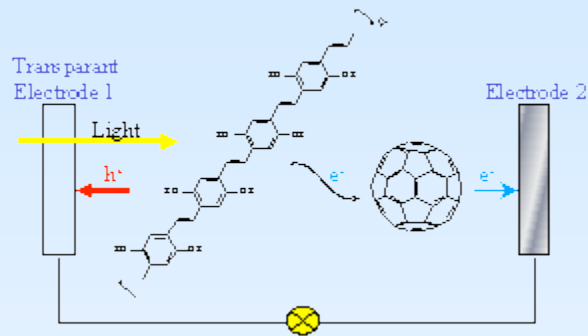


Scalable, but not as efficient



HELIOS

Mass Production Solar Cells?

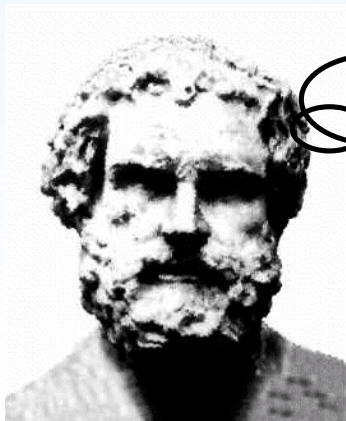
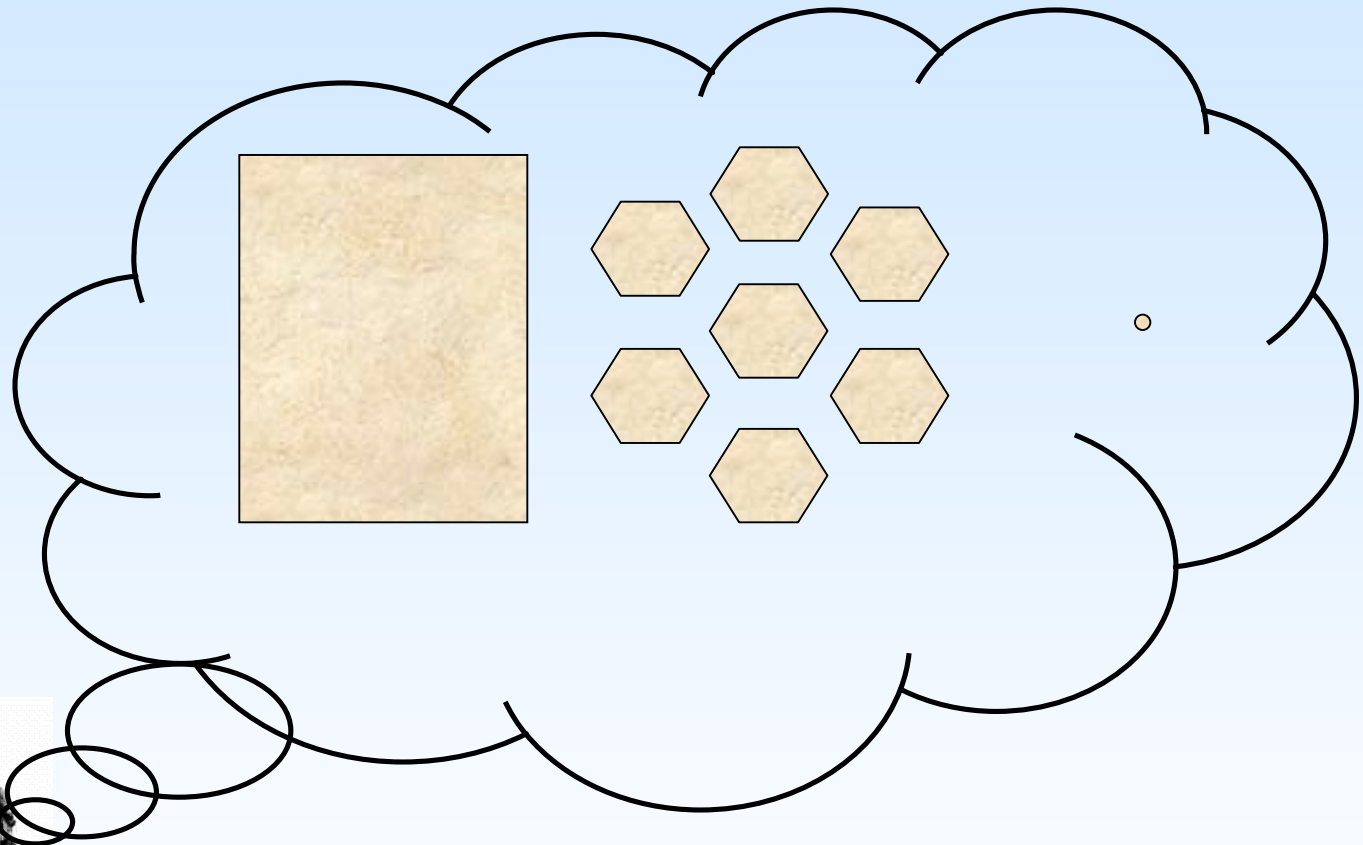


Let's take a look at nanotechnology



HELIOS

Democritus conceived of the atom...



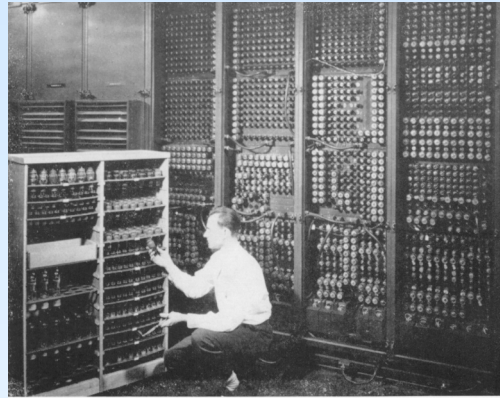
460-370 BC

...through successive division

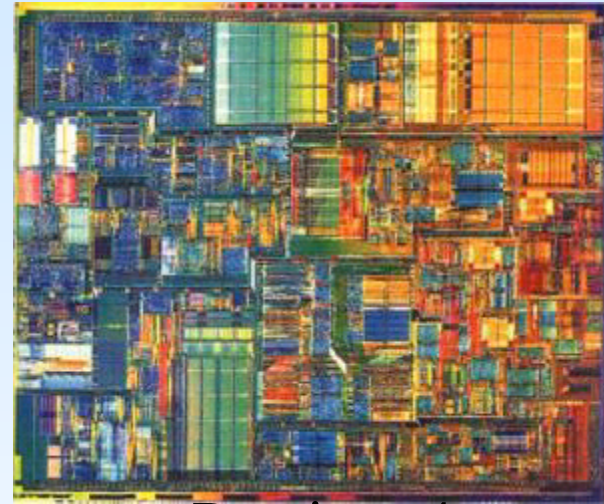
A modern version of Democritus' experiment



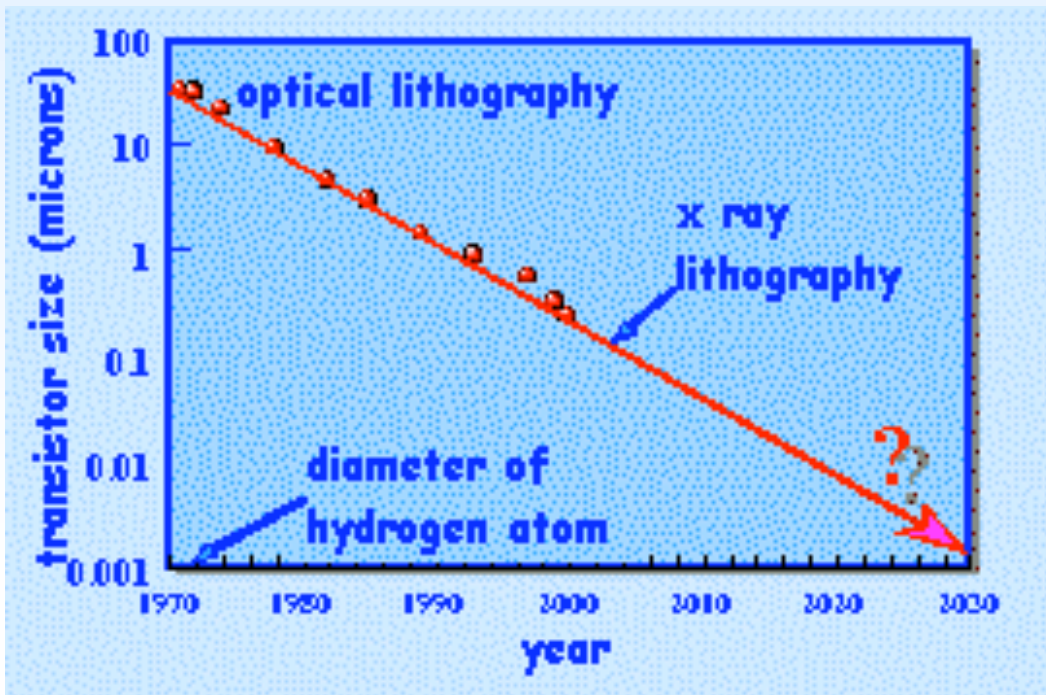
Gordon Moore



Replacing a bad tube meant checking among ENIAC's 19,000 possibilities.



Pentium 4





SCALING LAWS for nanocrystal properties



Melting temperature

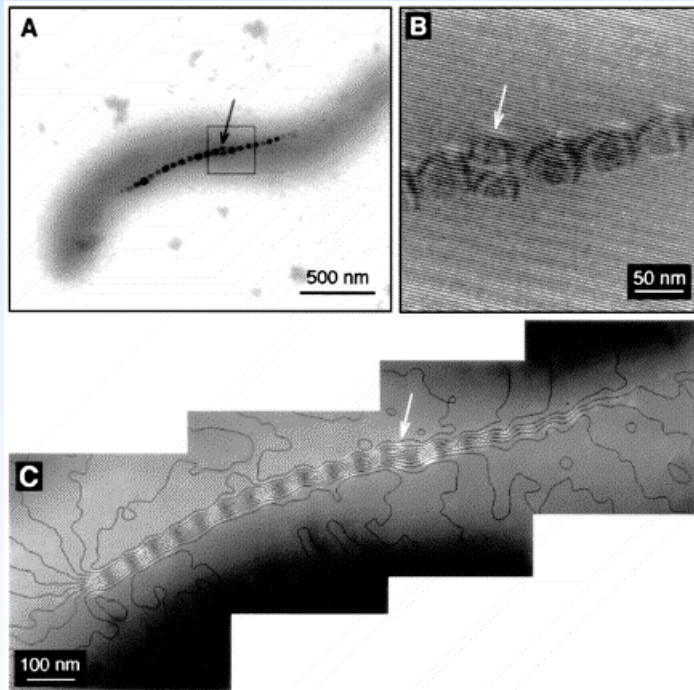
Band Gap and energy level spacing

Hardness

Magnetism...

Control of size and shape on the nanoscale opens
a third dimension to the periodic table

Nanocrystals and the exploitation of scaling laws ubiquitous in nature: example Magnetotactic Bacteria



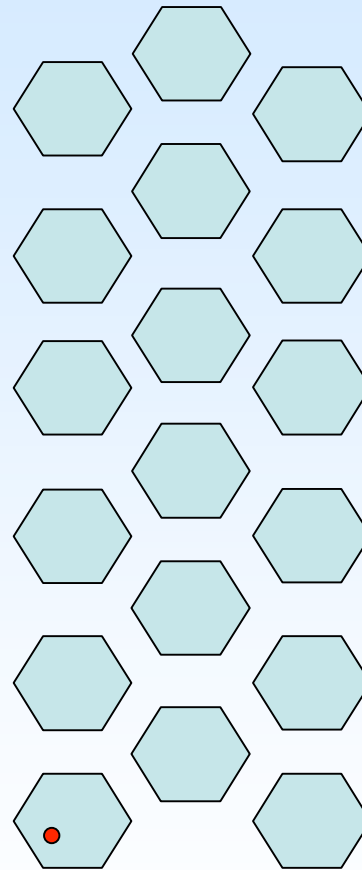
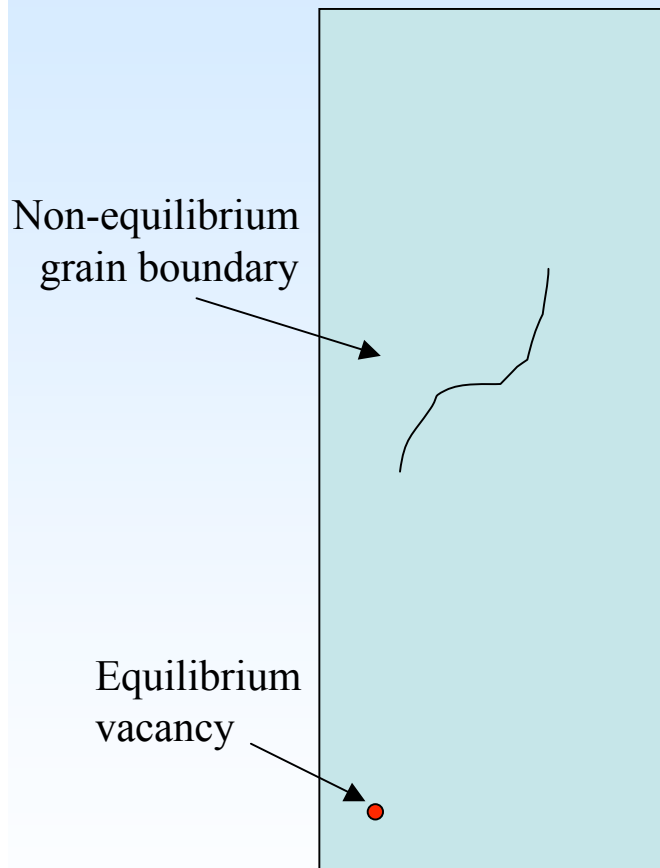
- Exploitation of a fundamental scaling law
- Maximum size for a magnet to be a “single domain,” with no defects (tens of nm)
- Least amount of material to achieve the greatest degree of magnetization.

Magnetospirillum magnetotacticum

TEM images from Frankel, R. B., Bazylinski, D. A., et. al.

Science **1998**, 282, 1868-1870

A comparison of defects in extended solids and nanocrystals



- 1 defect can affect an entire bulk solid
- On average, nanocrystals contain no equilibrium defects
- Easier to anneal out non-equilibrium defects in nanocrystals



From the de Beers educational web site:

“Big diamonds are much rarer, so a diamond of double the weight costs around 4 times more.”

Thermal motion



HELIOS

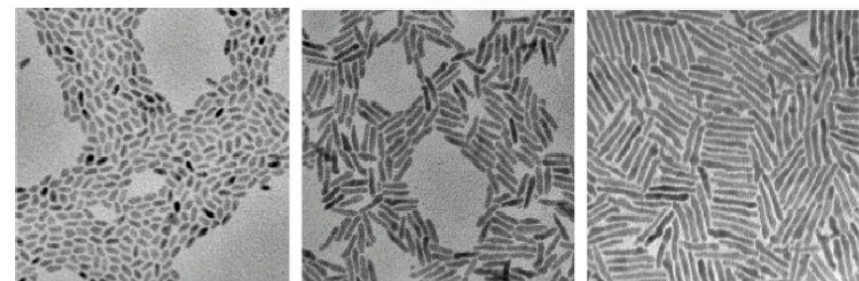
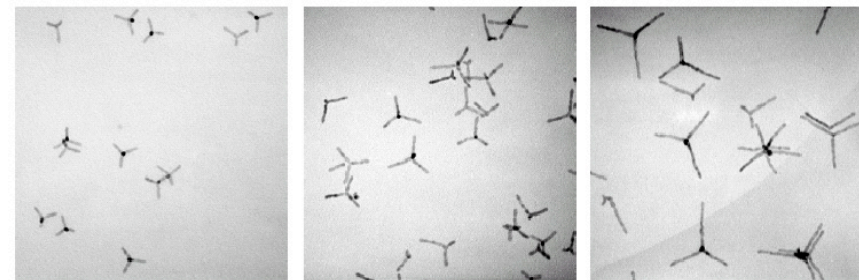
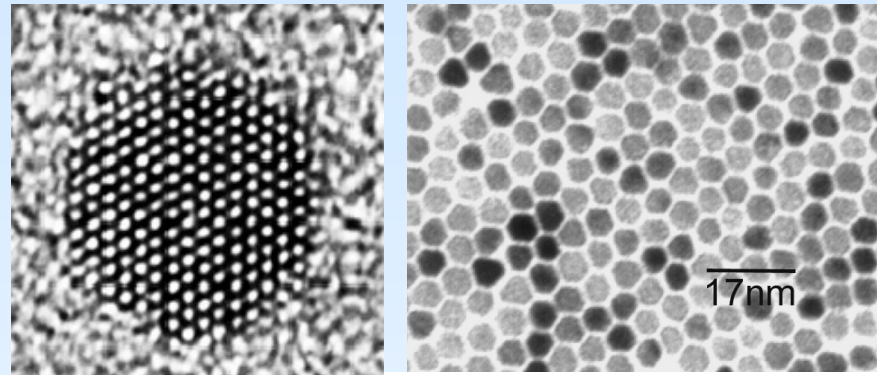
Big crystals vs. Nanocrystals



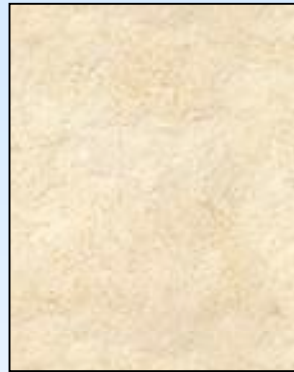
- Size: .000002- .000200 mm



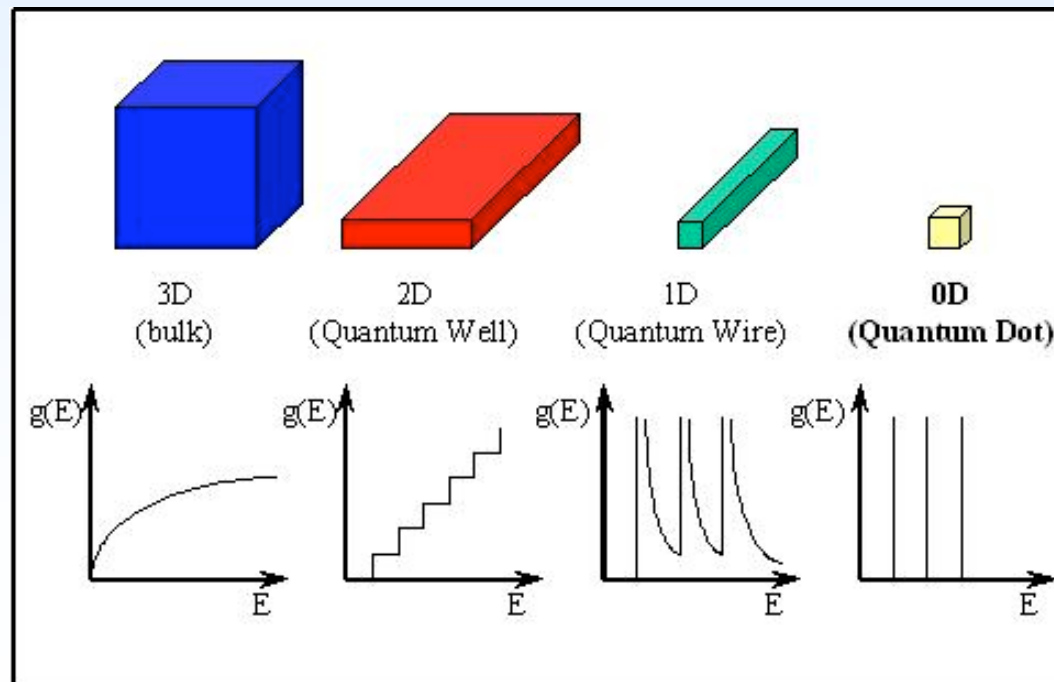
A crystal of silicon grown by the Czochralski (CZ) process can take from days to weeks



Electron energy levels in solids, nanocrystals, and atoms

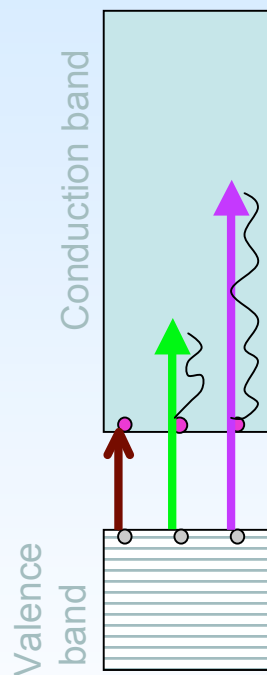


continuous

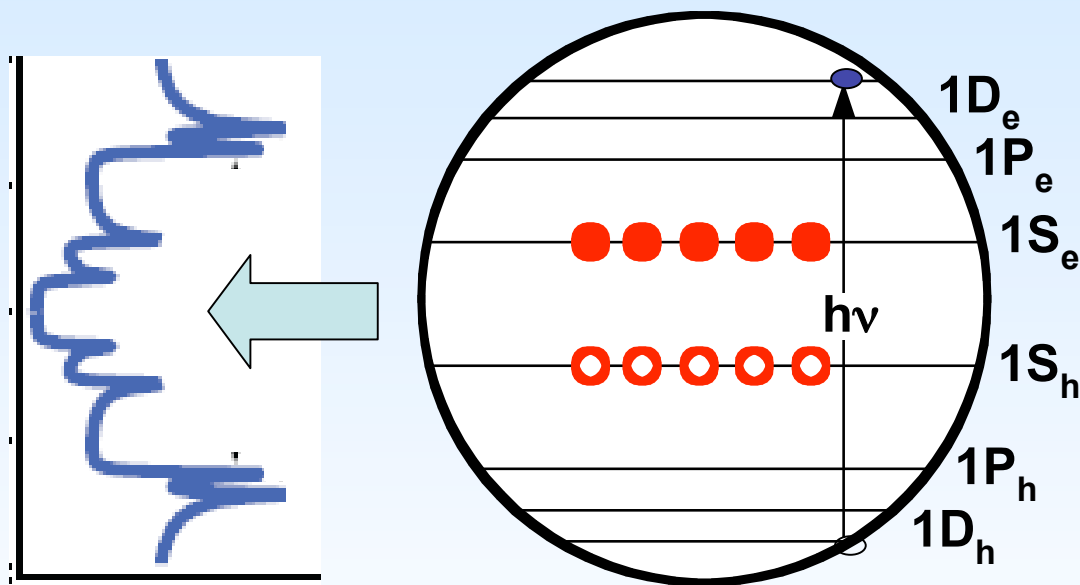


discrete

Schemes for harvesting solar energy more efficiently



“bulk crystal”

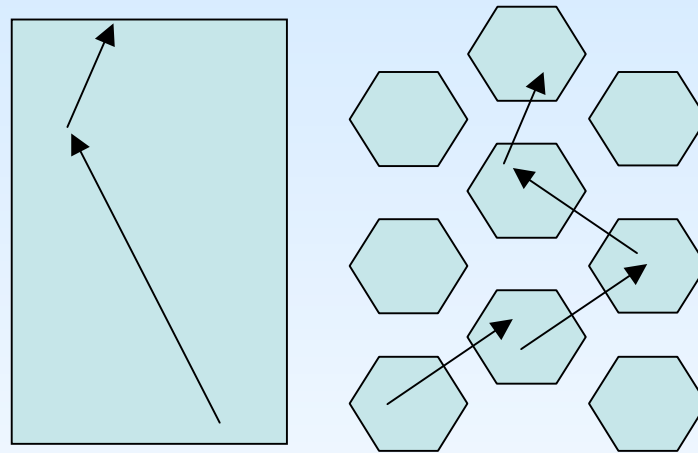


nanocrystal coupled to nanowire



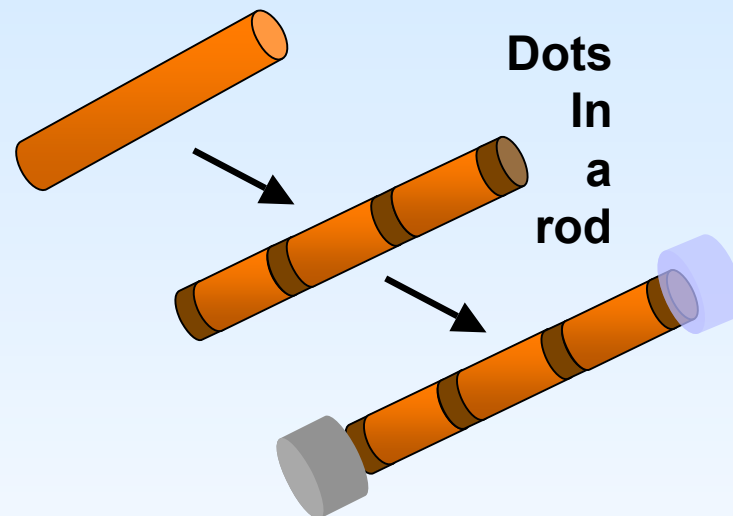
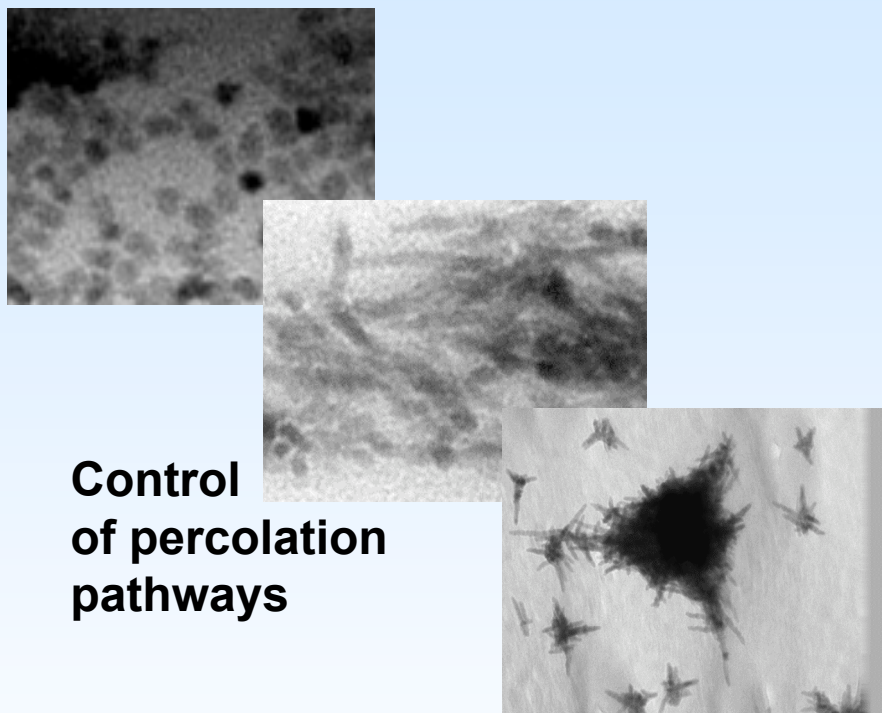
HELIOS

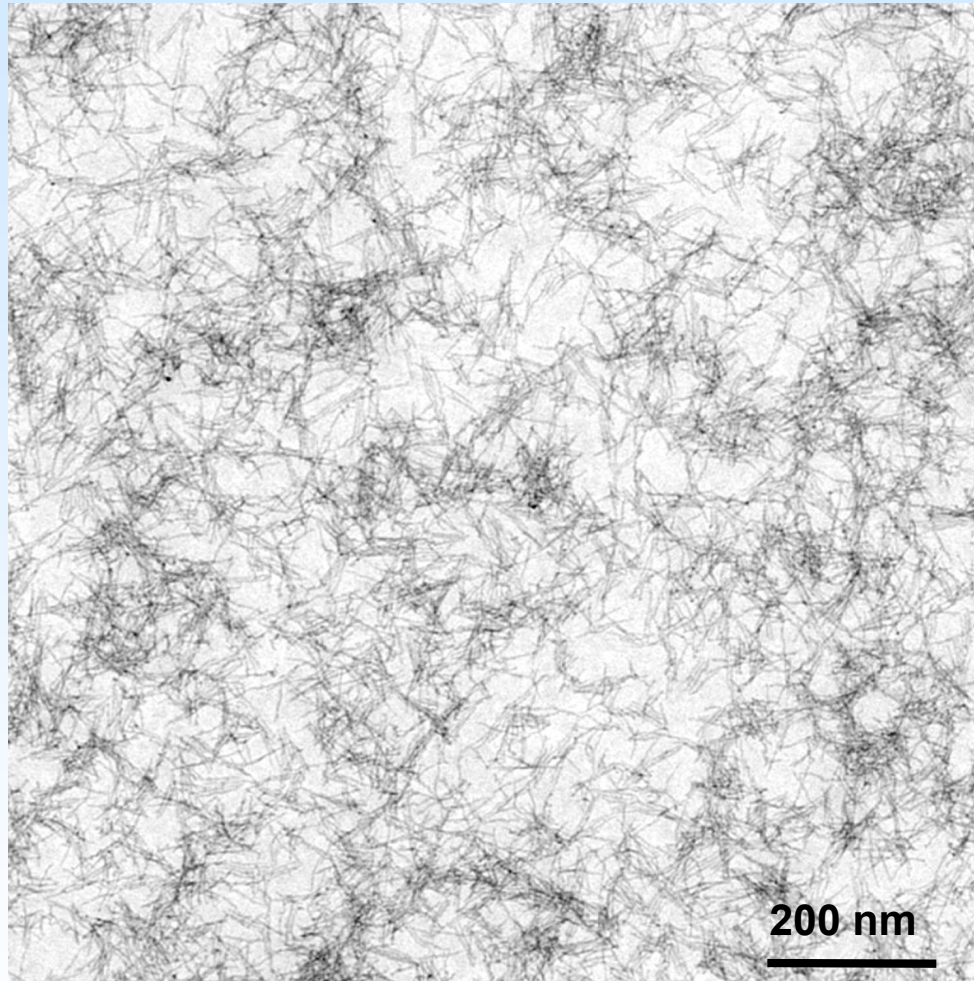
The problem of collecting charges in nano PVs



- Large number of interfaces and vastly greater surface area
- Potential for charge trapping and carrier loss

Studies of some nanocrystal-based solar cells





spin cast from solvent

Huynh, W. U., J. J. Dittmer, W. C. Libby, G. L. Whiting and A. P. Alivisatos (2003).

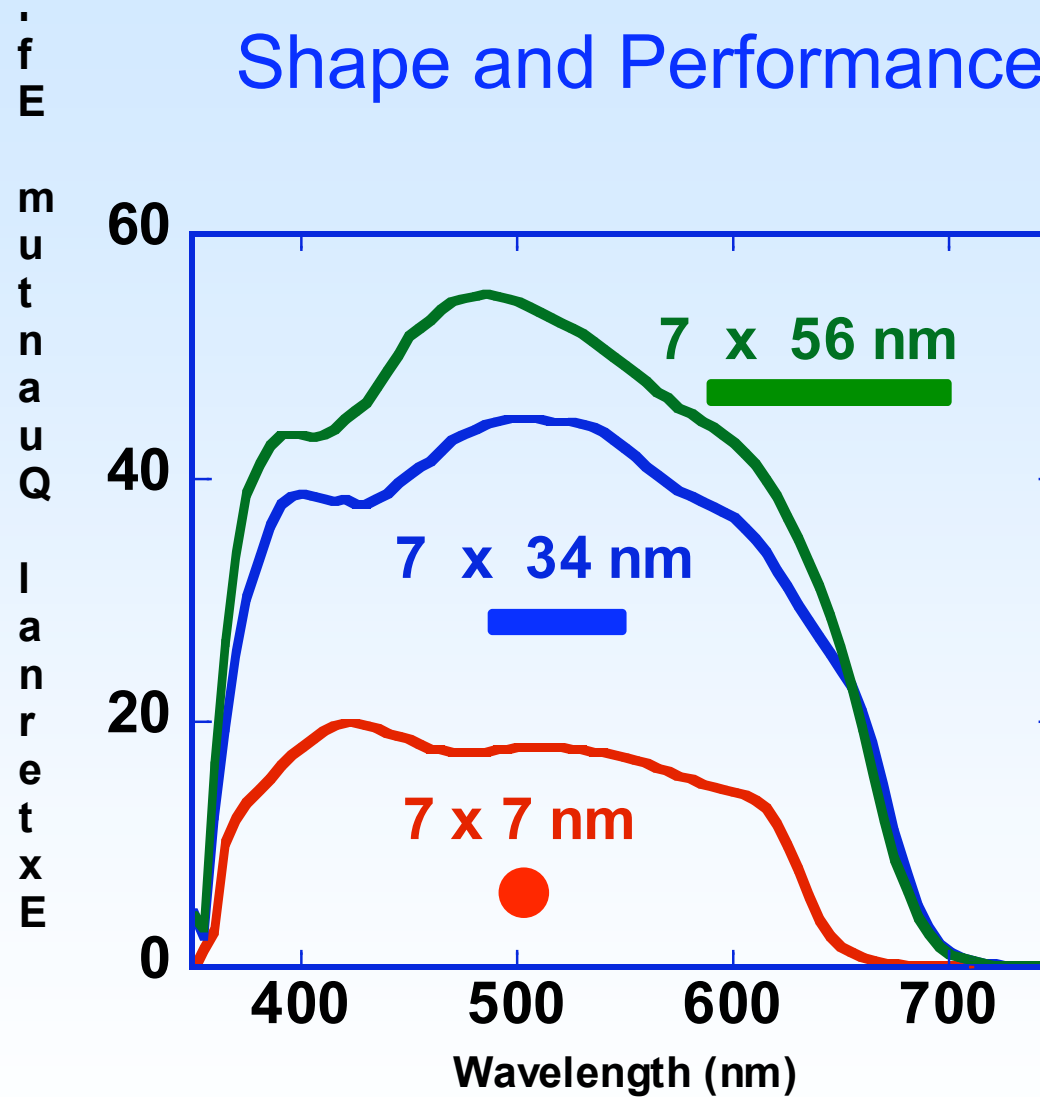
"Controlling the morphology of nanocrystal-polymer composites for solar cells." Advanced Functional Materials **13**(1): 73-79.



HELIOS



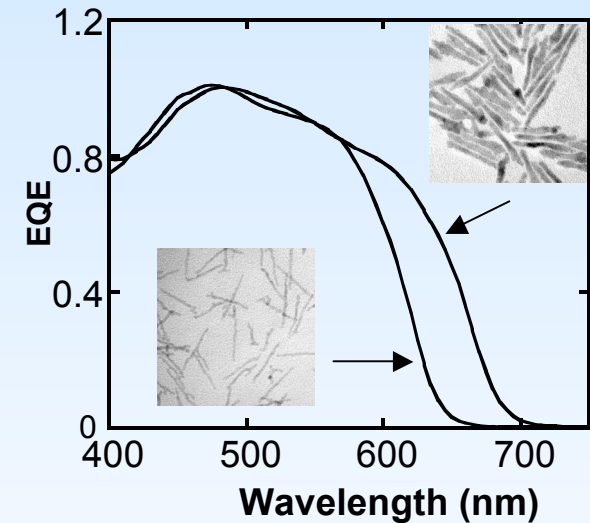
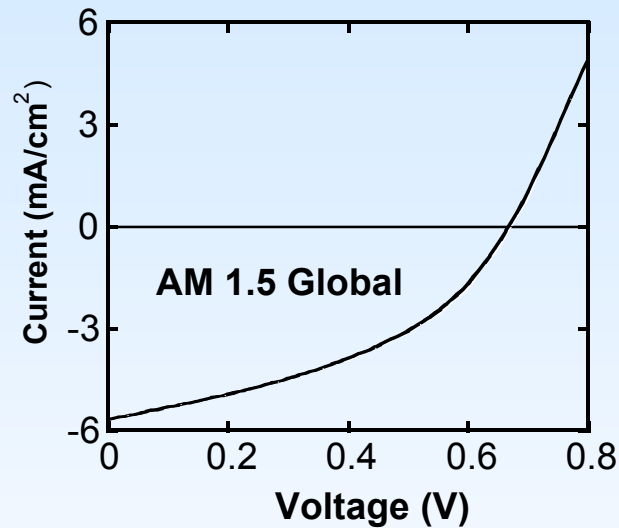
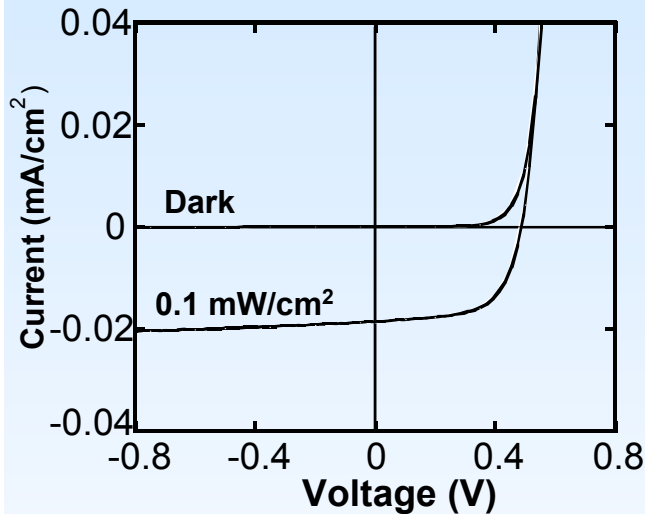
Shape and Performance



Measured at low intensity $\sim 0.1 \text{ mW/cm}^2$



Plastic/Nanorod Solar Cell Power Efficiency



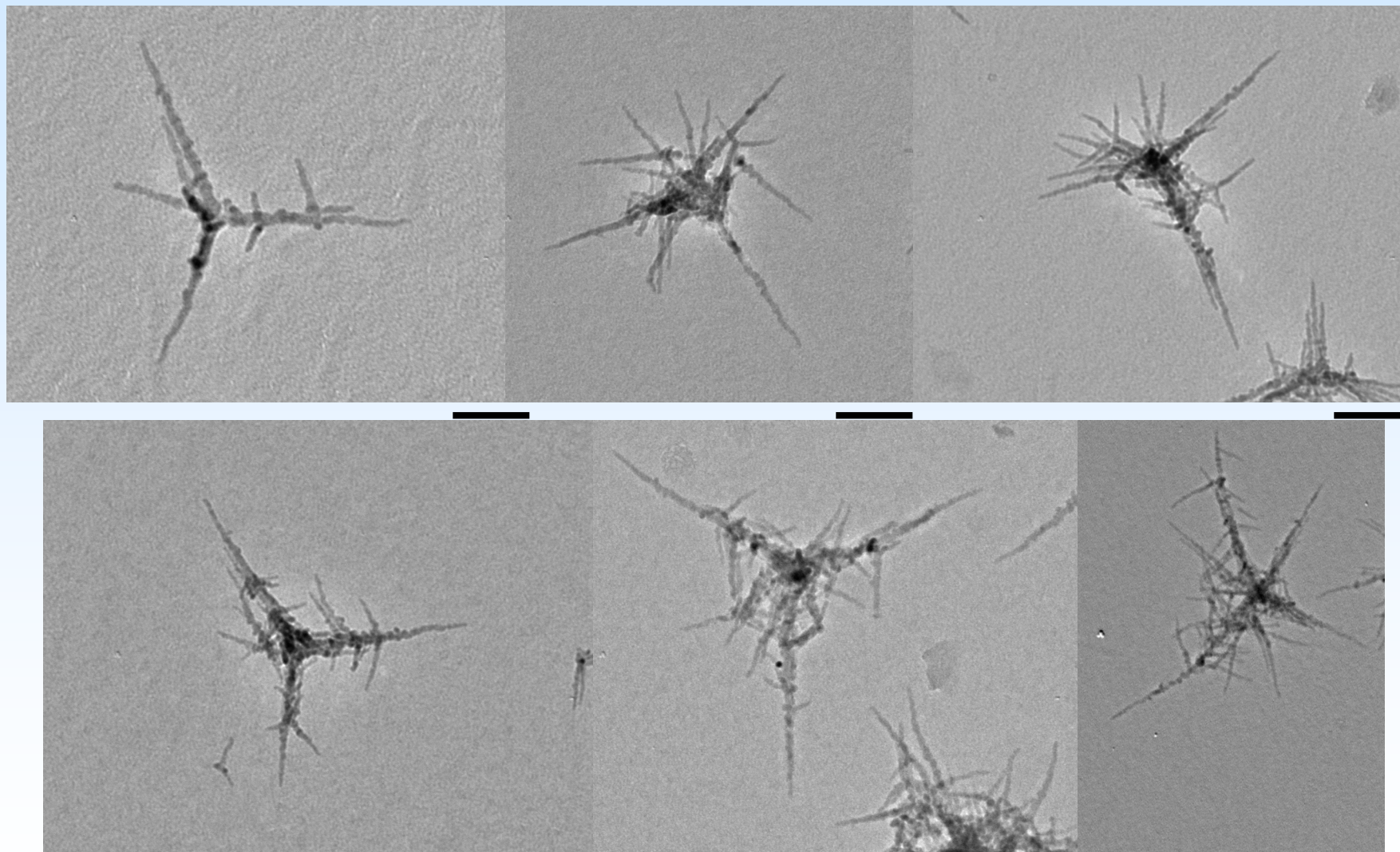
AM 1.5 Efficiency

Power Conversion: **1.7%**

Short Circuit Current: 5.8
mA/cm²

Fill Factor: 0.42

V_{oc} : 0.67 V



Kanaras, A. G., C. Sonnichsen, H. T. Liu and A. P. Alivisatos Nano Letters 5(11): 2164-2167. (2005).

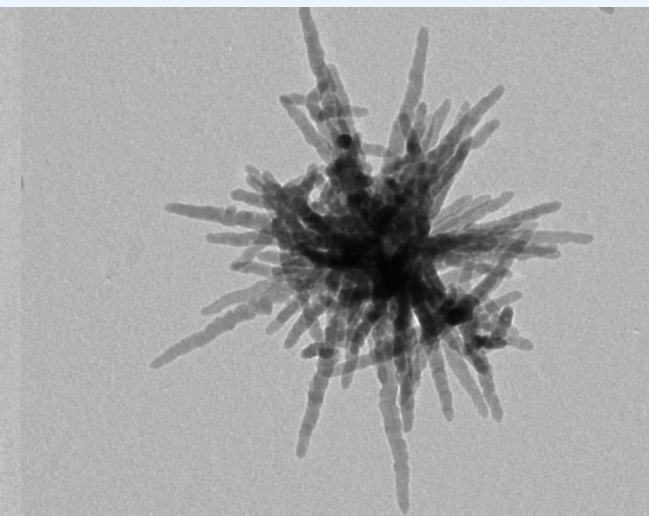
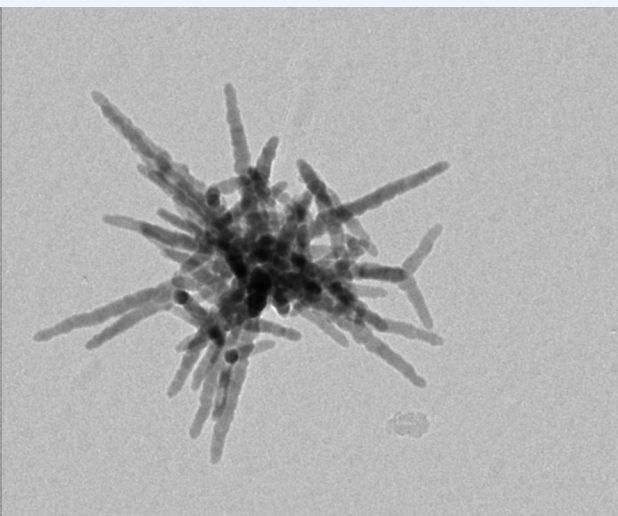
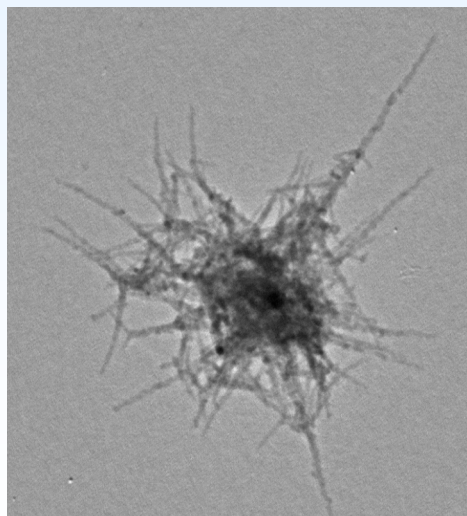
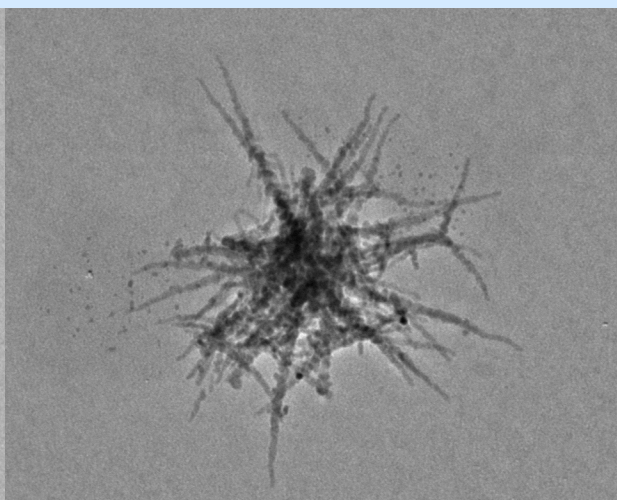
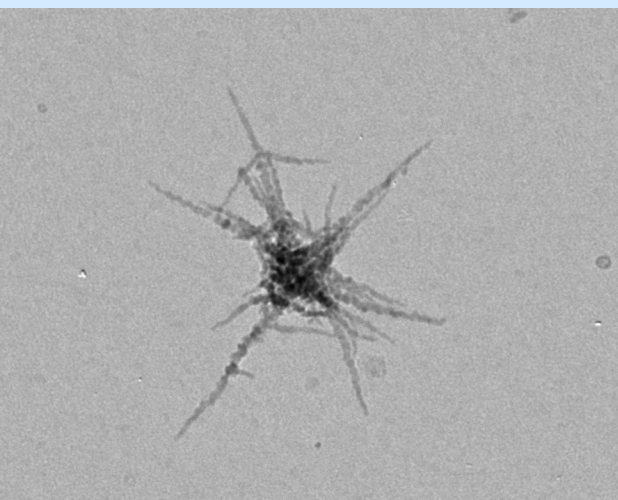
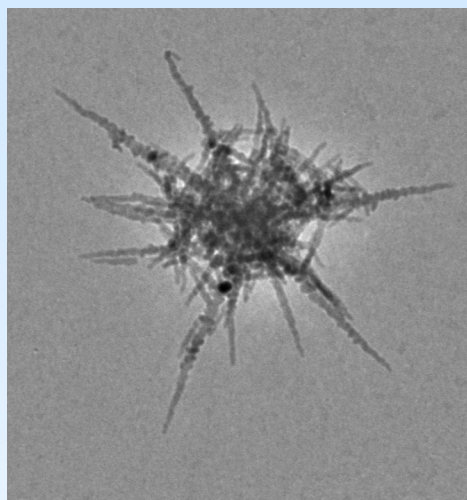
"Controlled synthesis of hyperbranched inorganic nanocrystals with rich three-dimensional structures."

100
nm



HELIOS

Branchy crystals –2nd aliquot

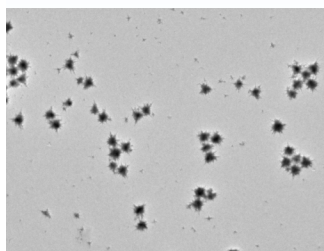
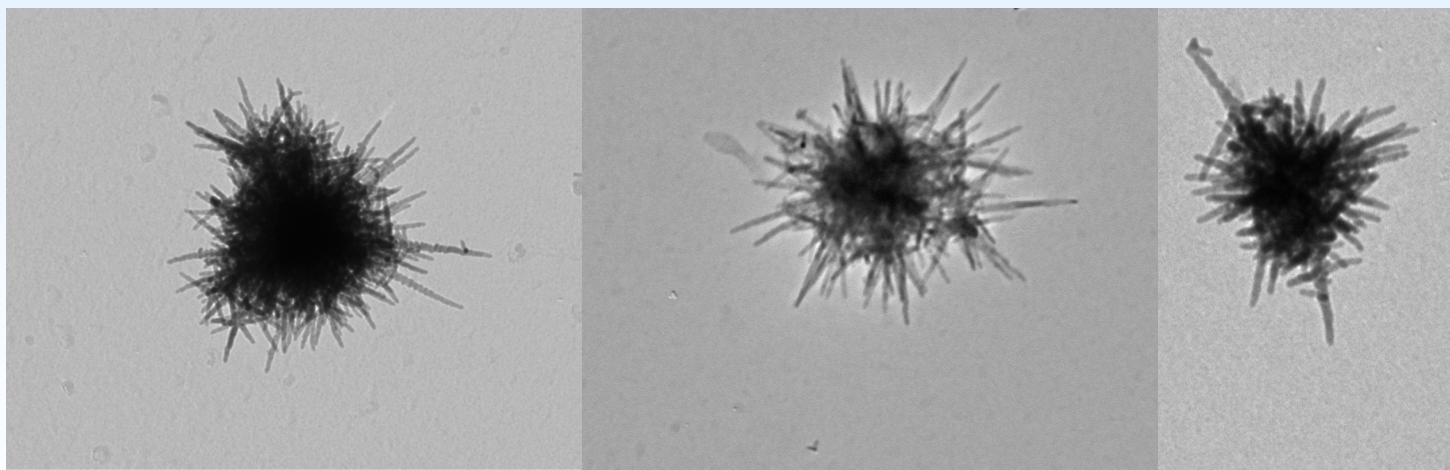
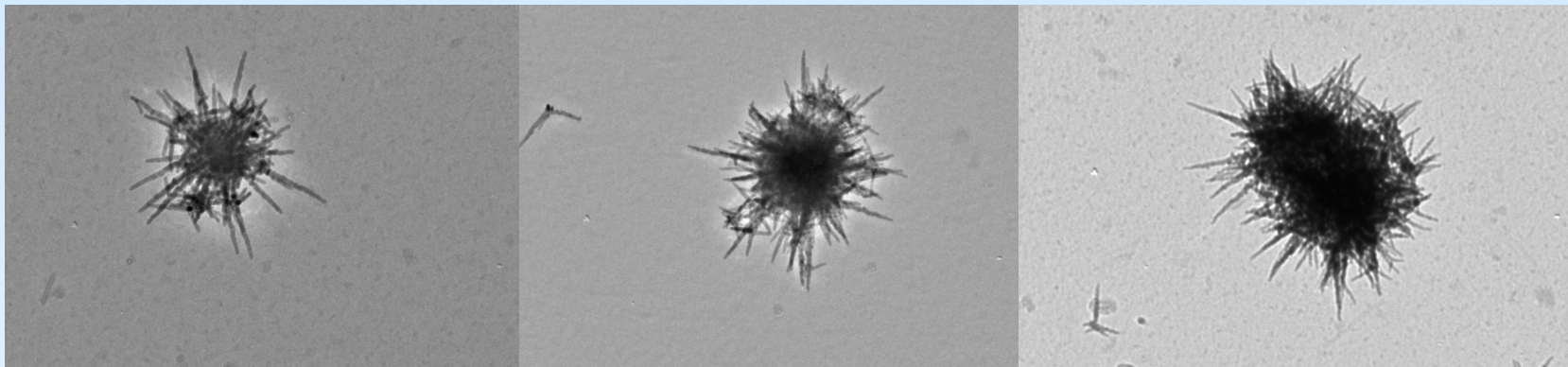


100 nm



HELIOS

Branchy crystals –3rd aliquot

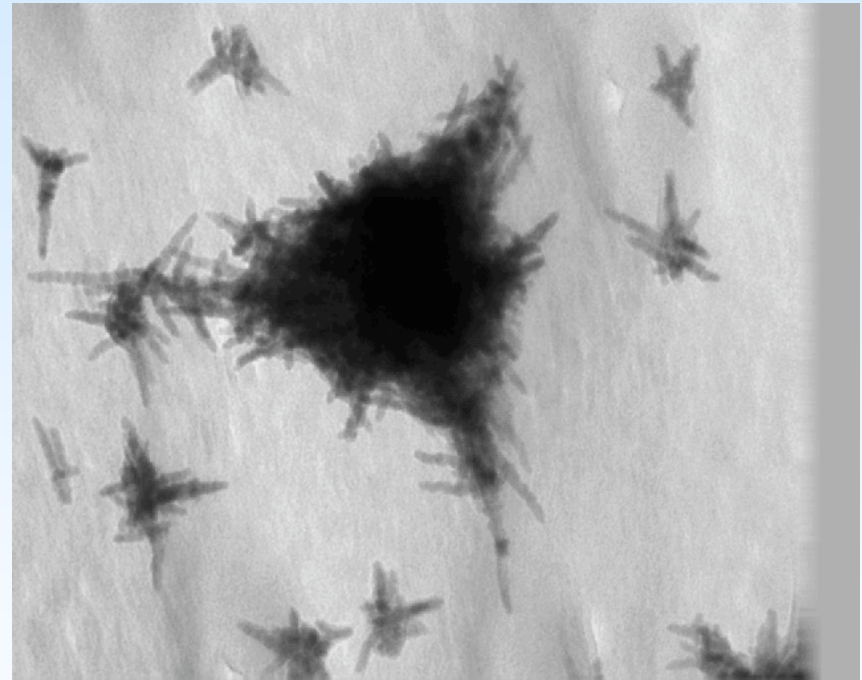
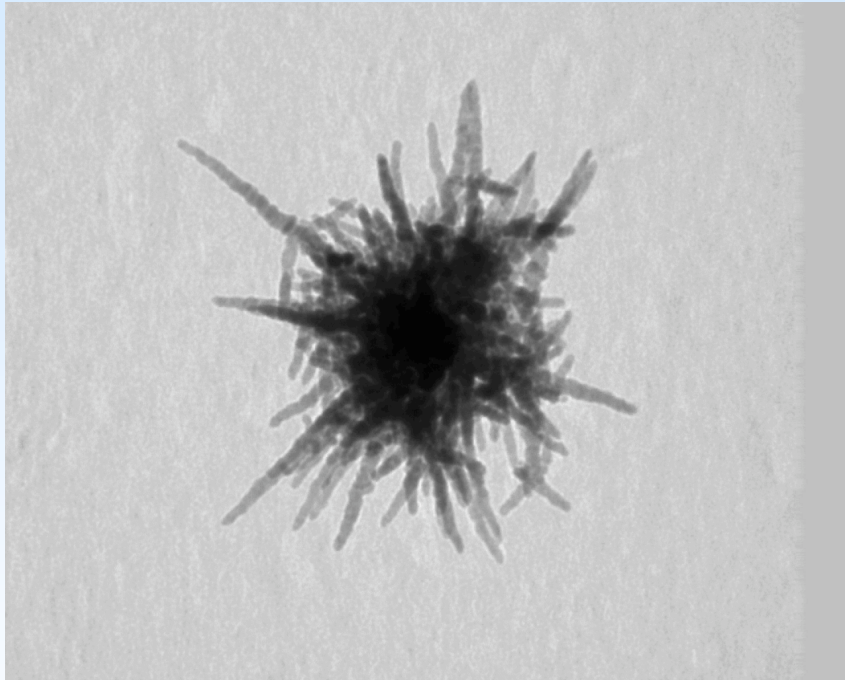


100 nm

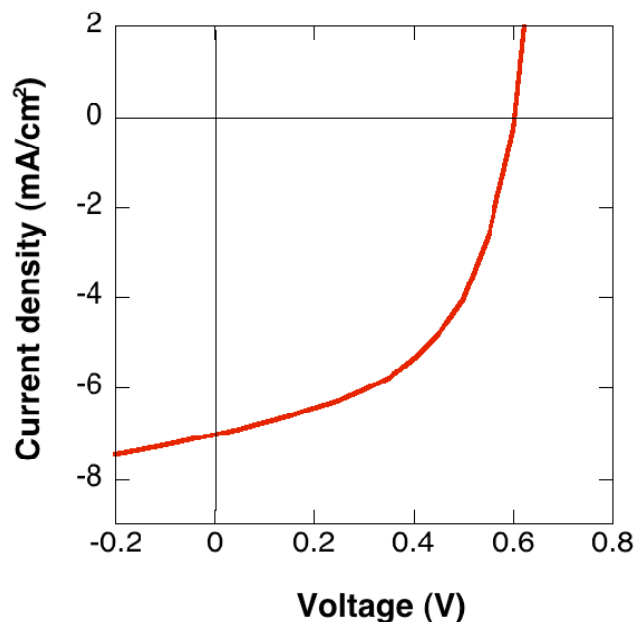
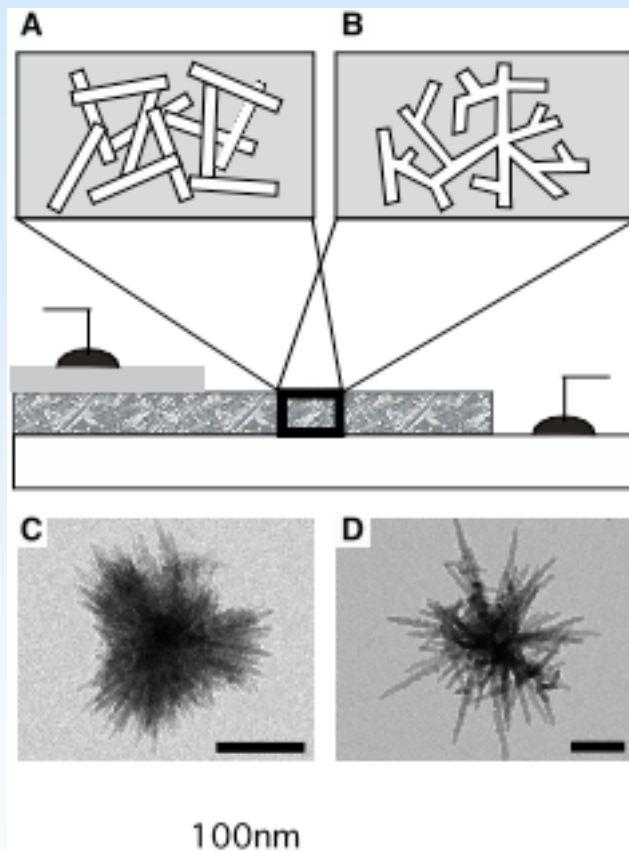
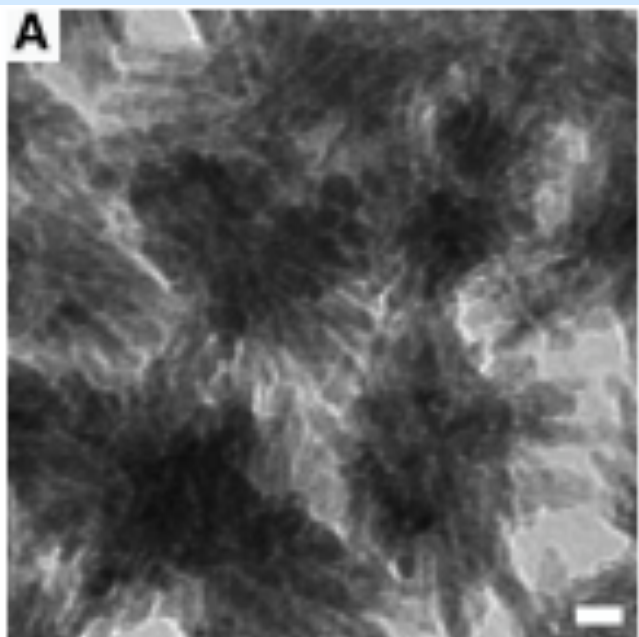


HELIOS

Tomography



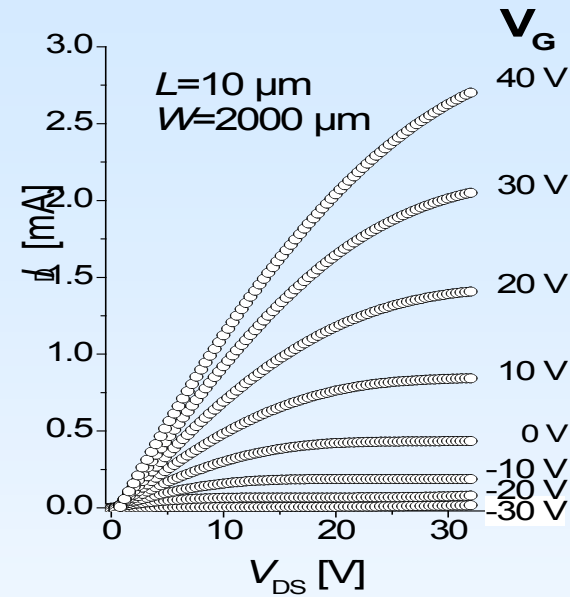
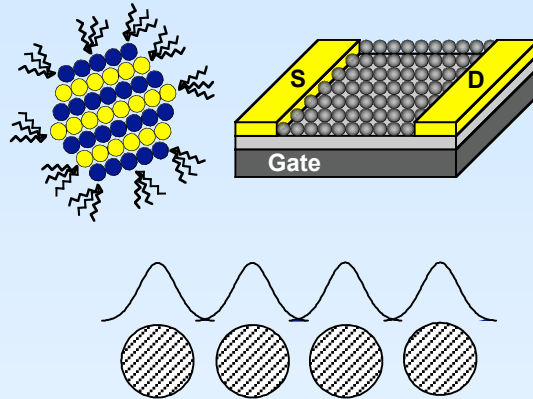
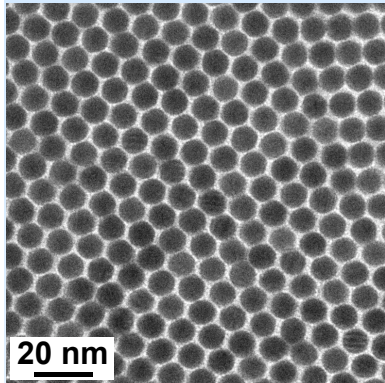
Pre-formed percolation pathways branched nanocrystals



~2.5 % Power Efficiency

Gur, N. A. Fromer, C. P. Chen, A. G. Kanaras, and A. P. Alivisatos, "Hybrid solar cells with prescribed nanoscale morphologies based on hyperbranched semiconductor nanocrystals," Nano Letters 7 (2), 409 (2007).

New approaches to balance confinement and transport

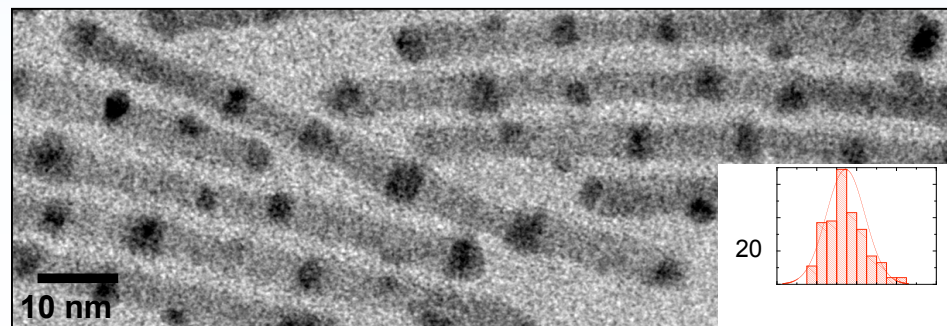
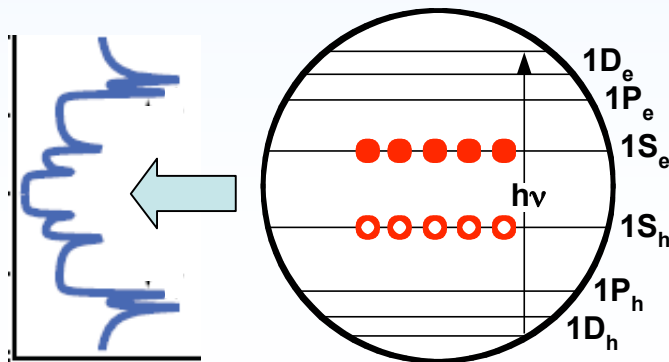
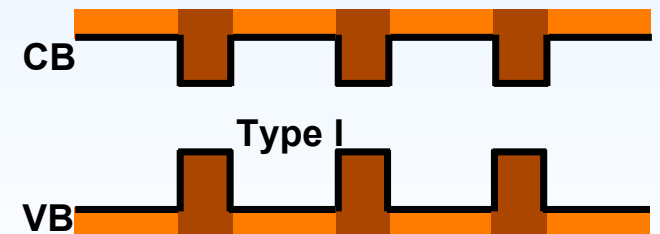
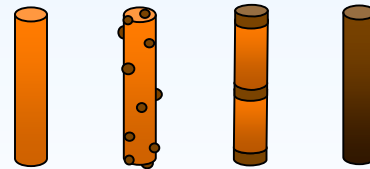


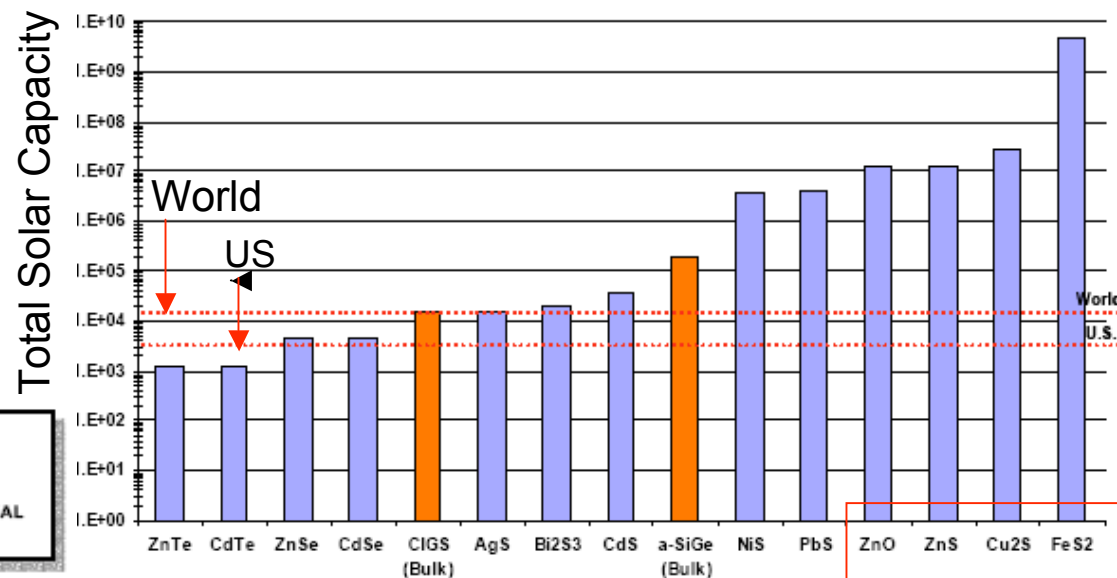
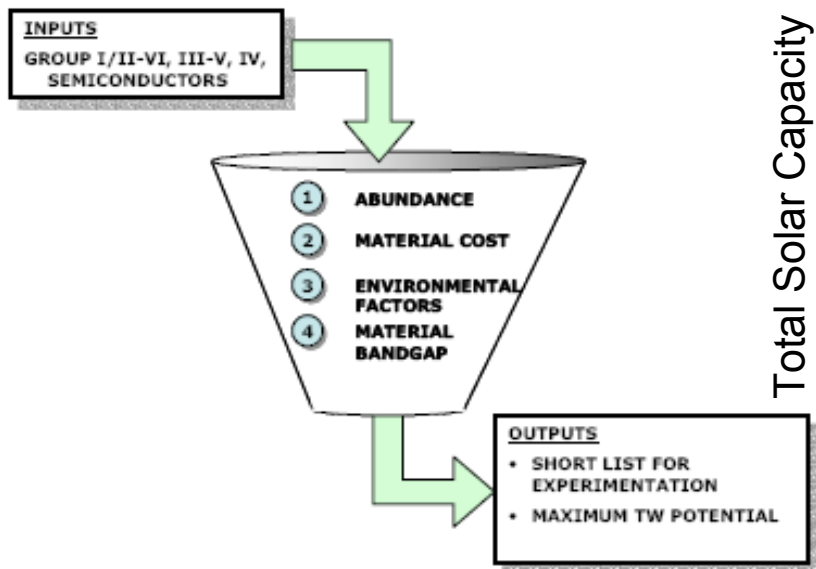
Mobility:
 $e^- 2.5\ \text{cm}^2\text{V}^{-1}\text{s}^{-1}$
 $h^+ 0.3\ \text{cm}^2\text{V}^{-1}\text{s}^{-1}$

D. Talapin,
 Science
 310 86 (2005)

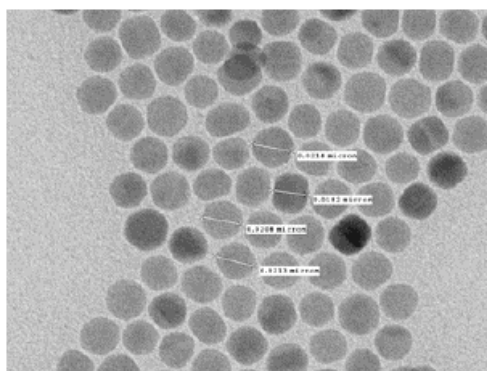
q dot superlattice
 treated with hydrazine

spontaneous formation
 of q dots in a rod

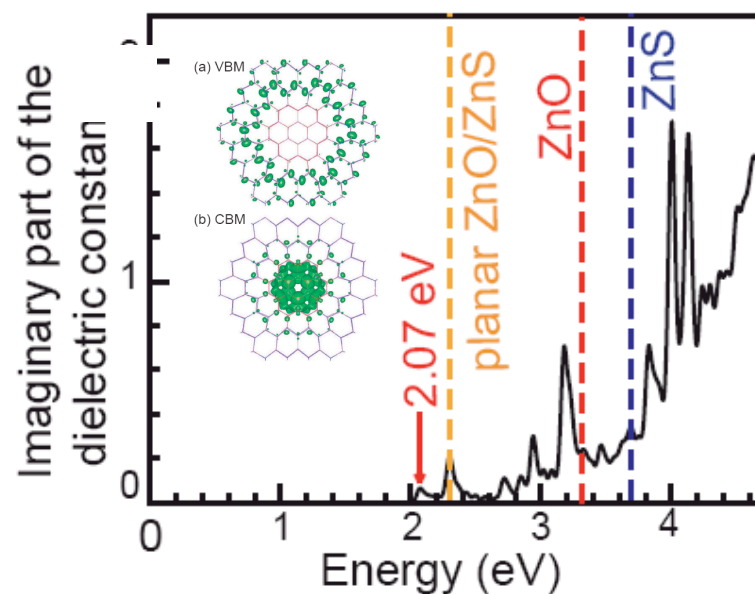
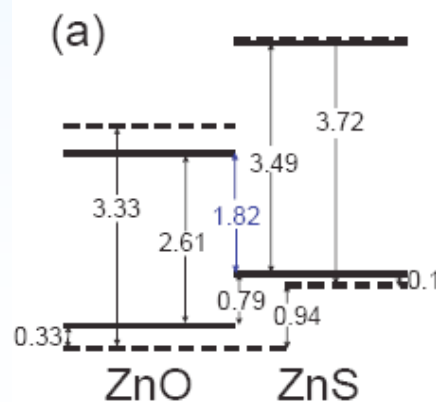




Cu₂S nanocrystals



001-185,018,117
200 kV
0.015 nm
11/07/05/15-05

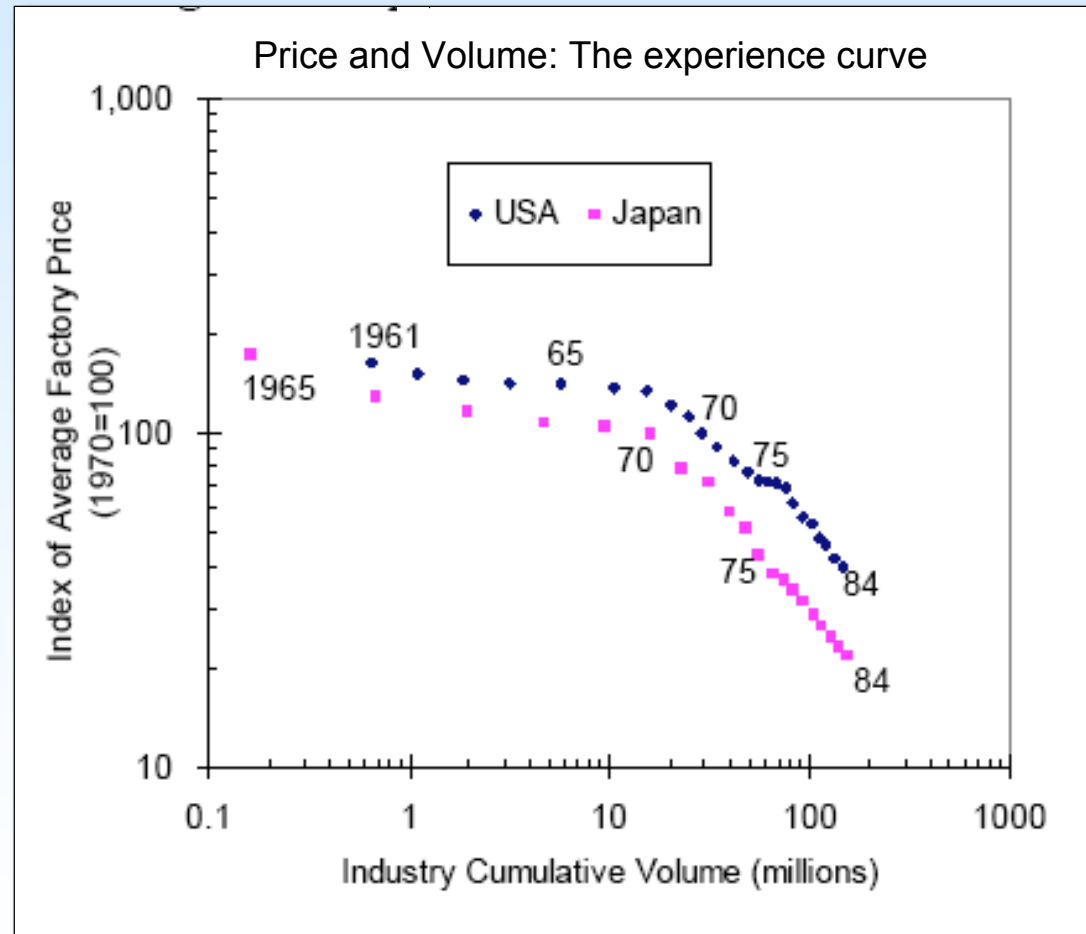
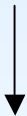




HELIOS



Vacuum tubes to transistors: History of Color TV '65-'85



Japanese learning rate: from 92.4% vs 61.1%



HELIOS

Could we jump to a new learning curve with nano PV?

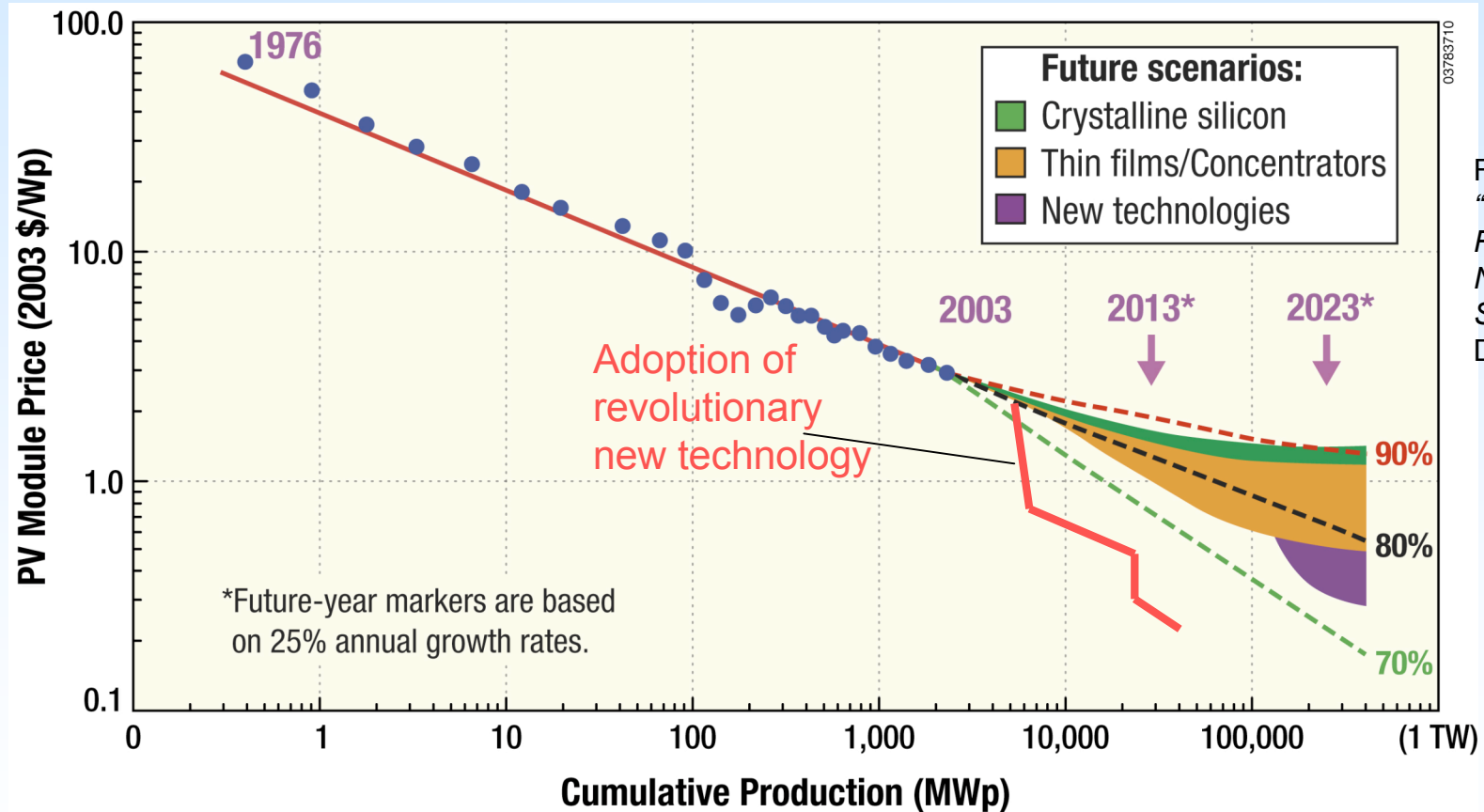
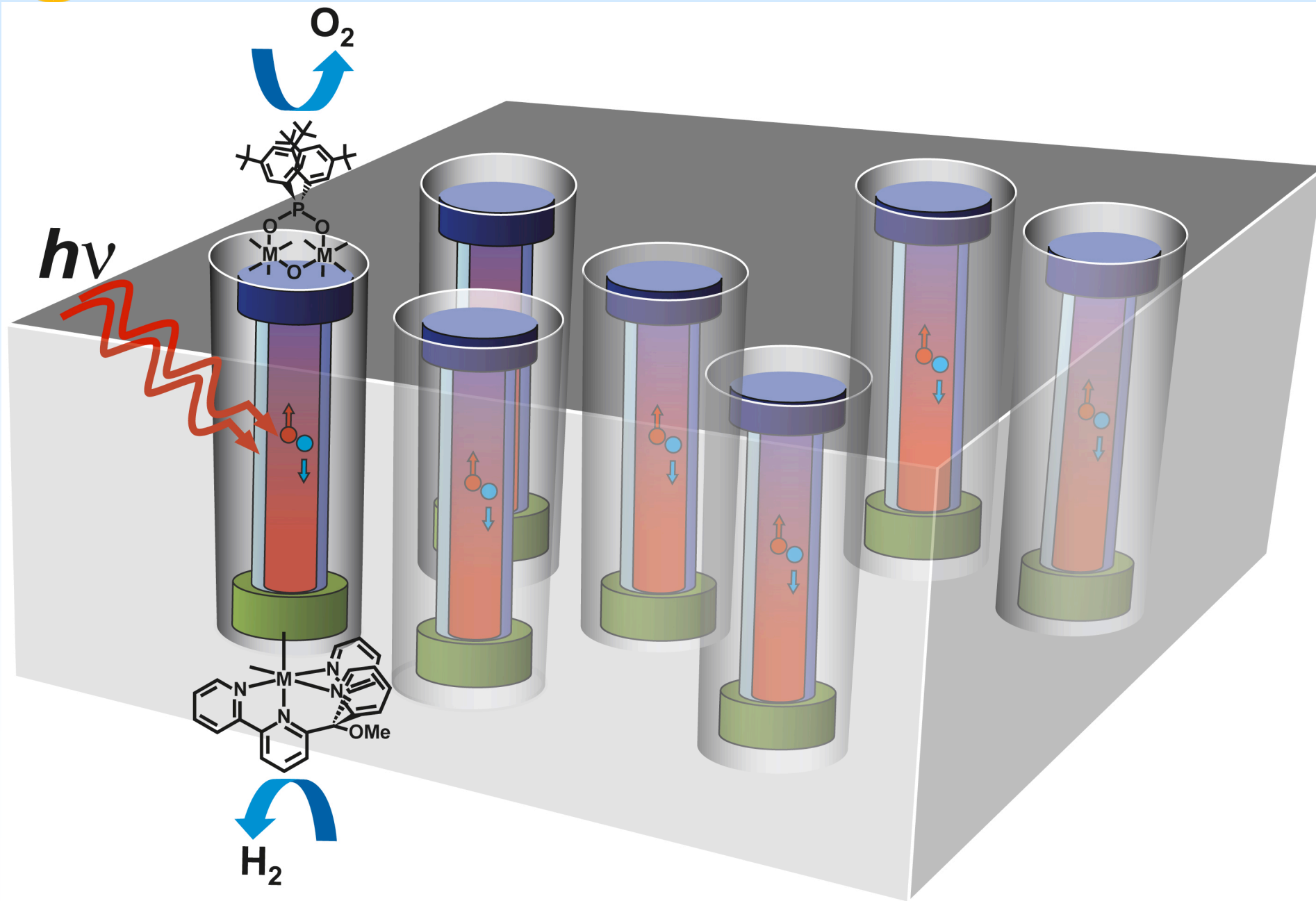


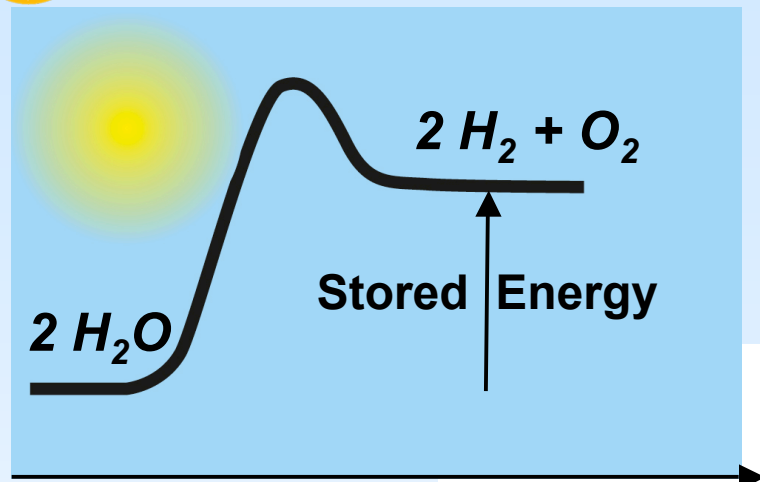
Figure from
"Basic
Research
Needs for
Solar Energy",
DOE, 2005



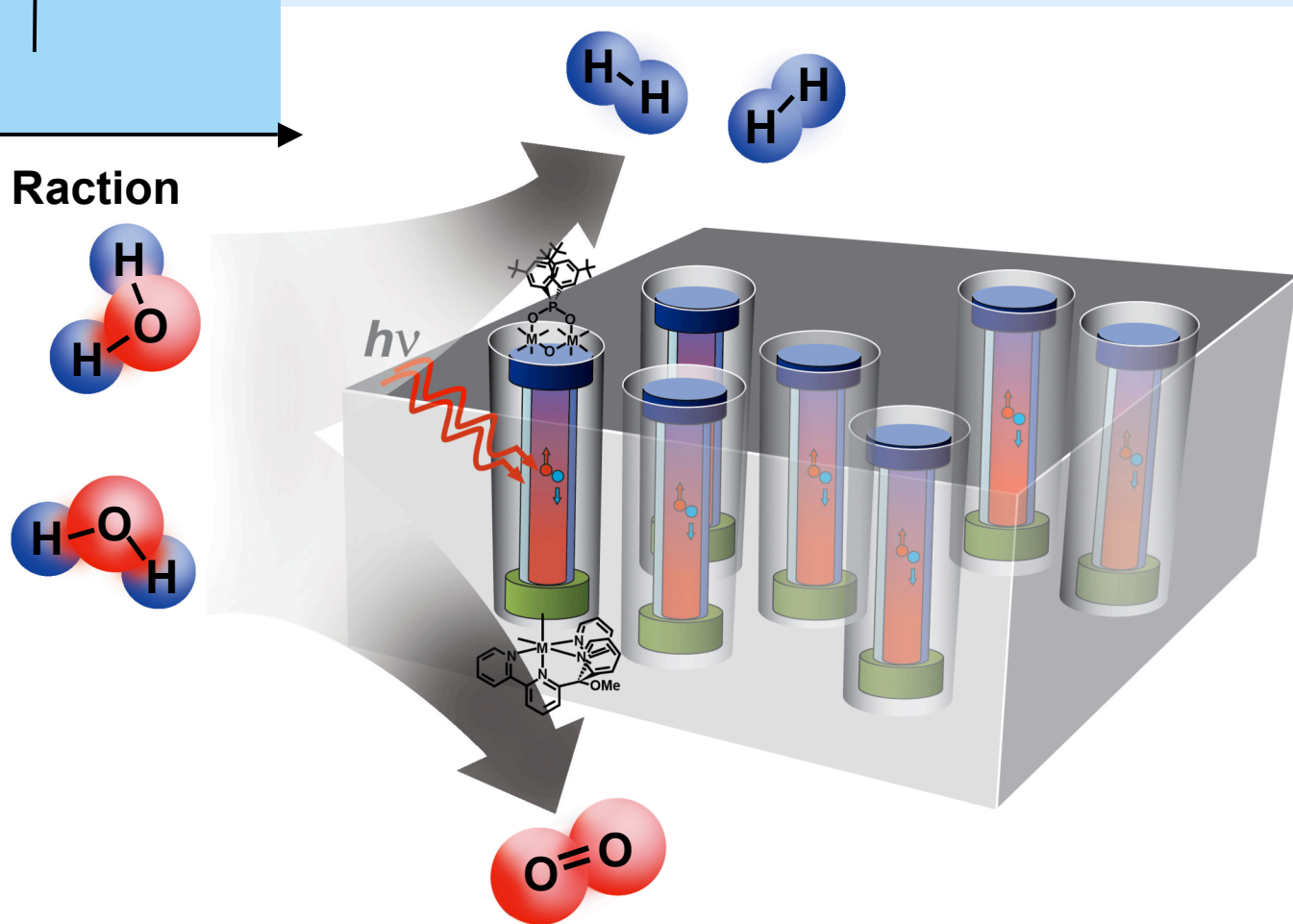
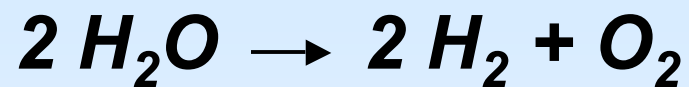


HELIOS

Water Splitting by Sunlight



Water Splitting Reaction

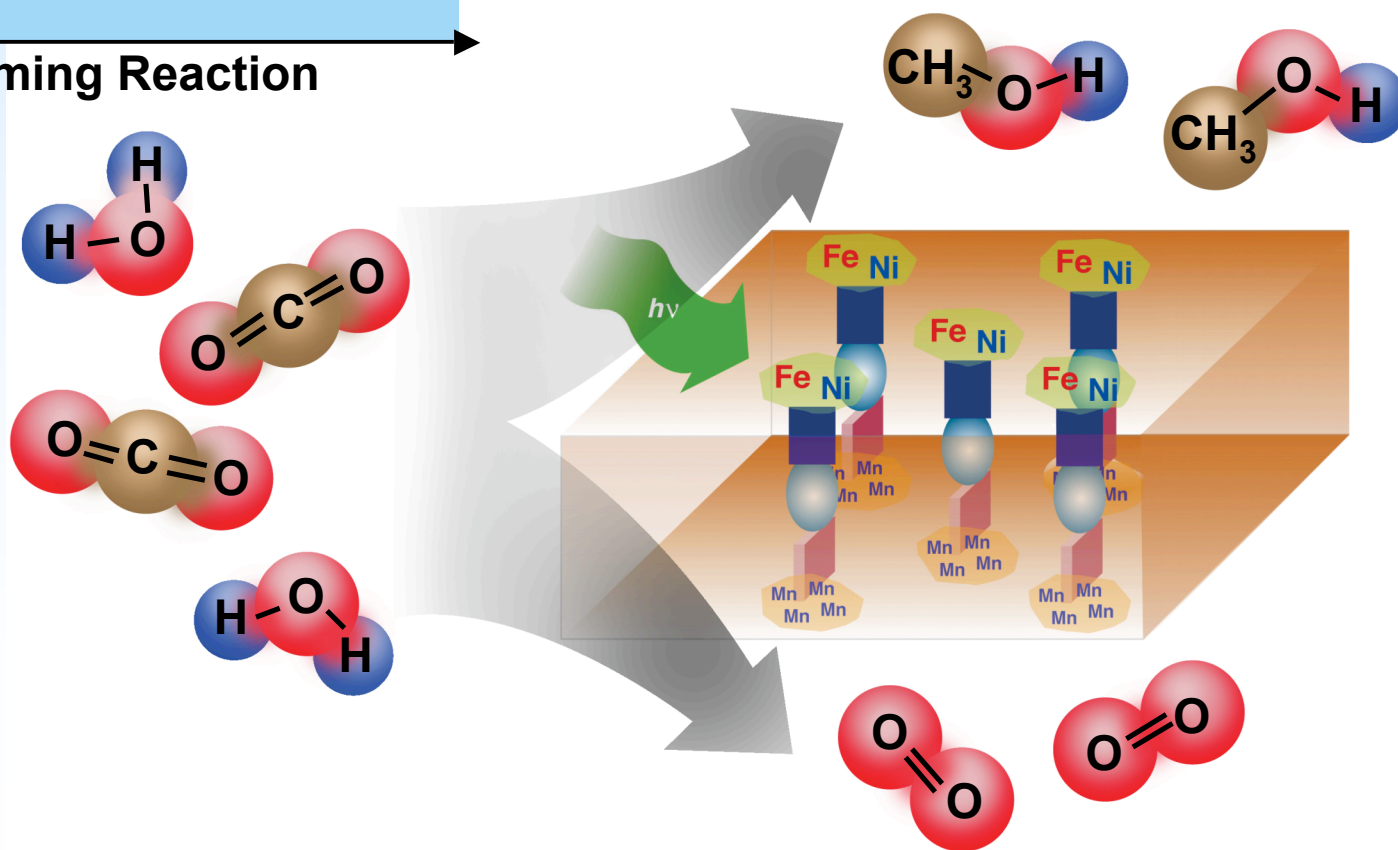
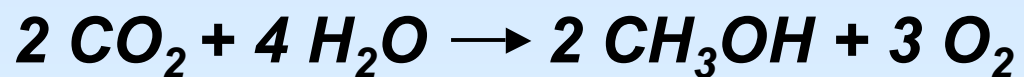
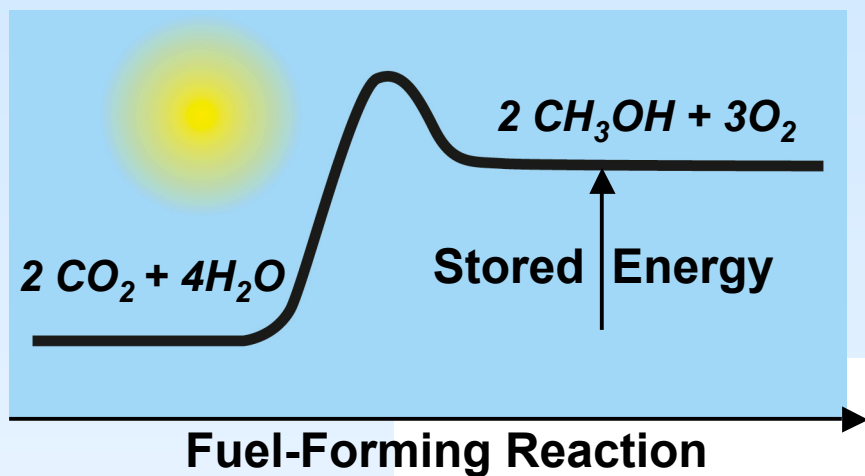




HELIOS

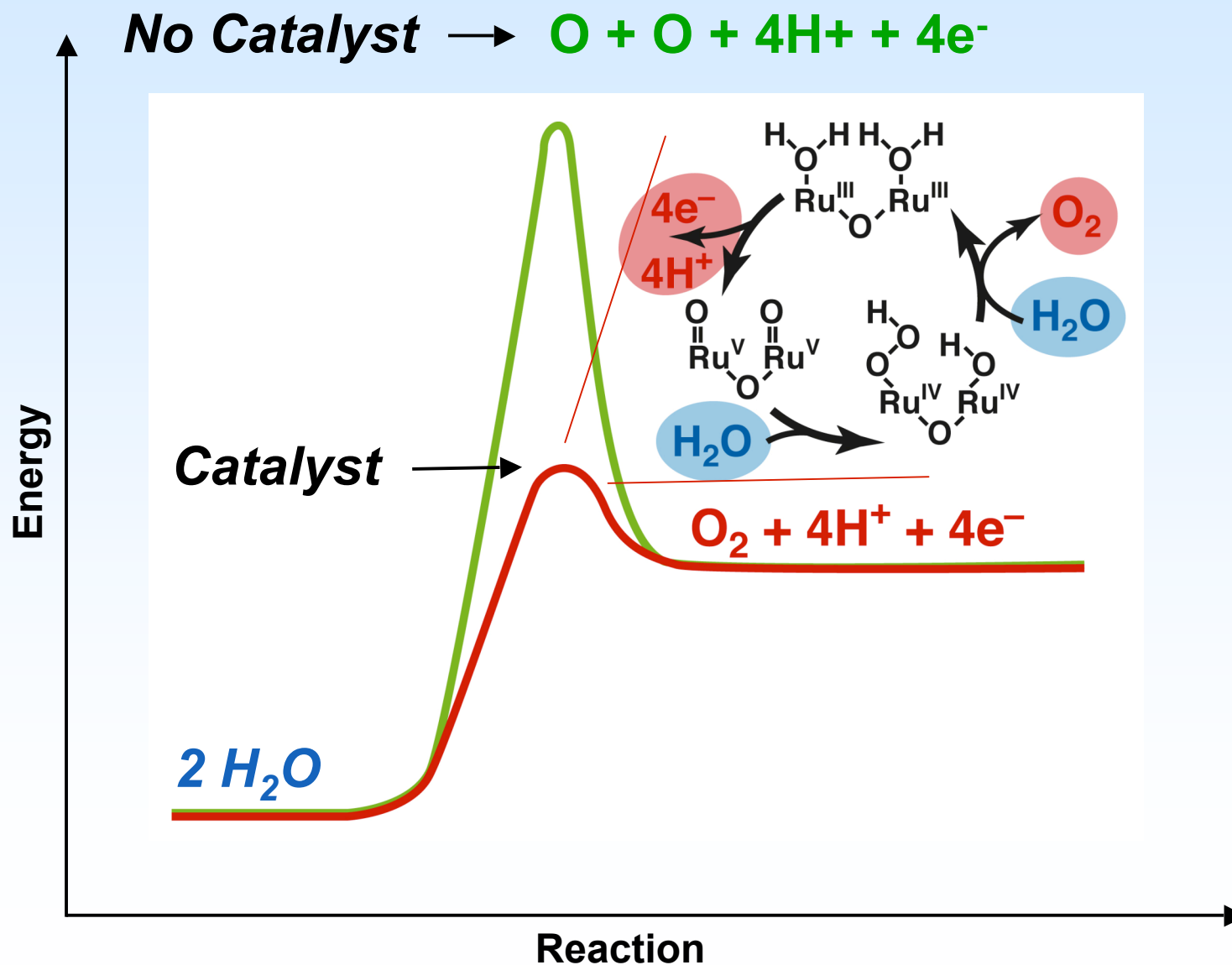


Carbon Dioxide to Liquid Fuel by Sunlight

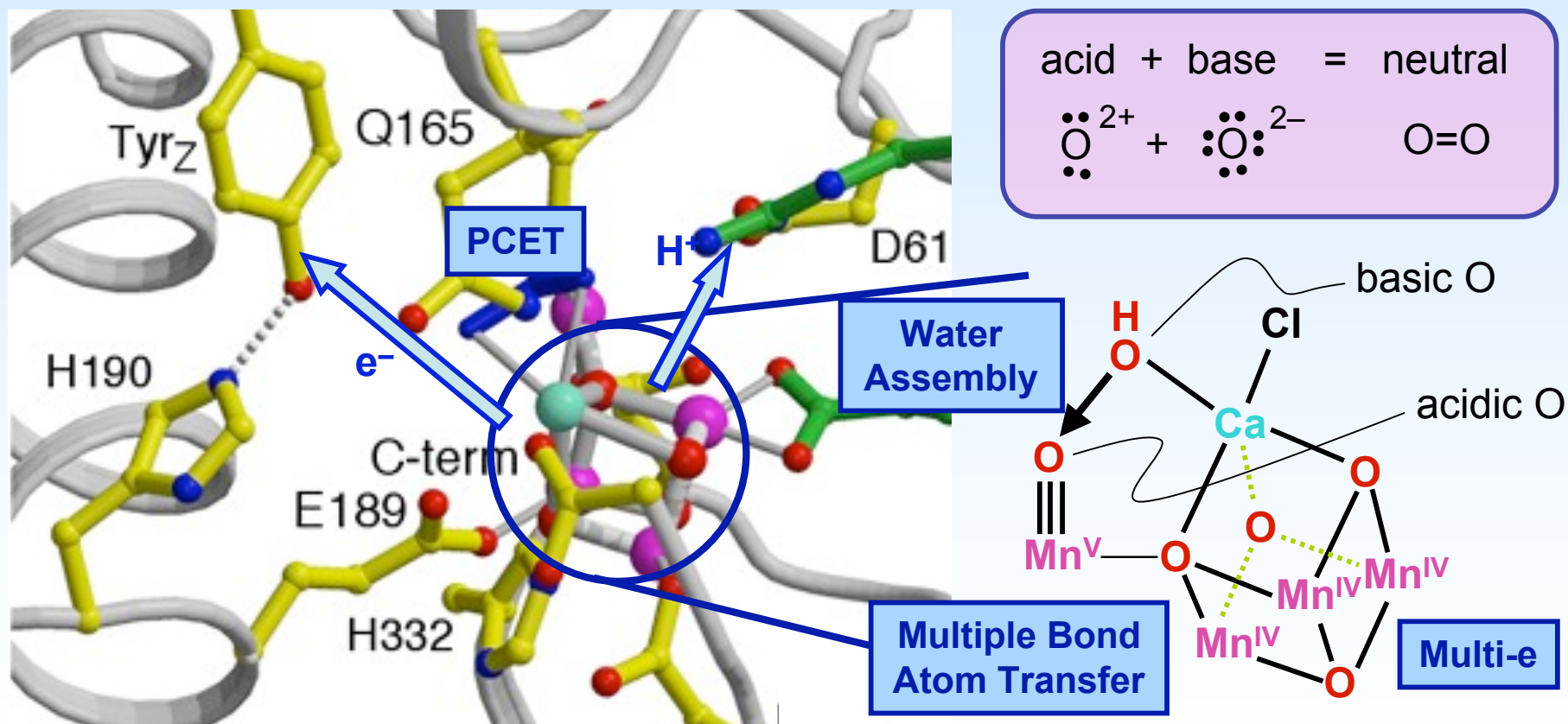


What a Catalyst Does

Example: Water Oxidation



The OEC Active Site of PSII (Imperial College structure)

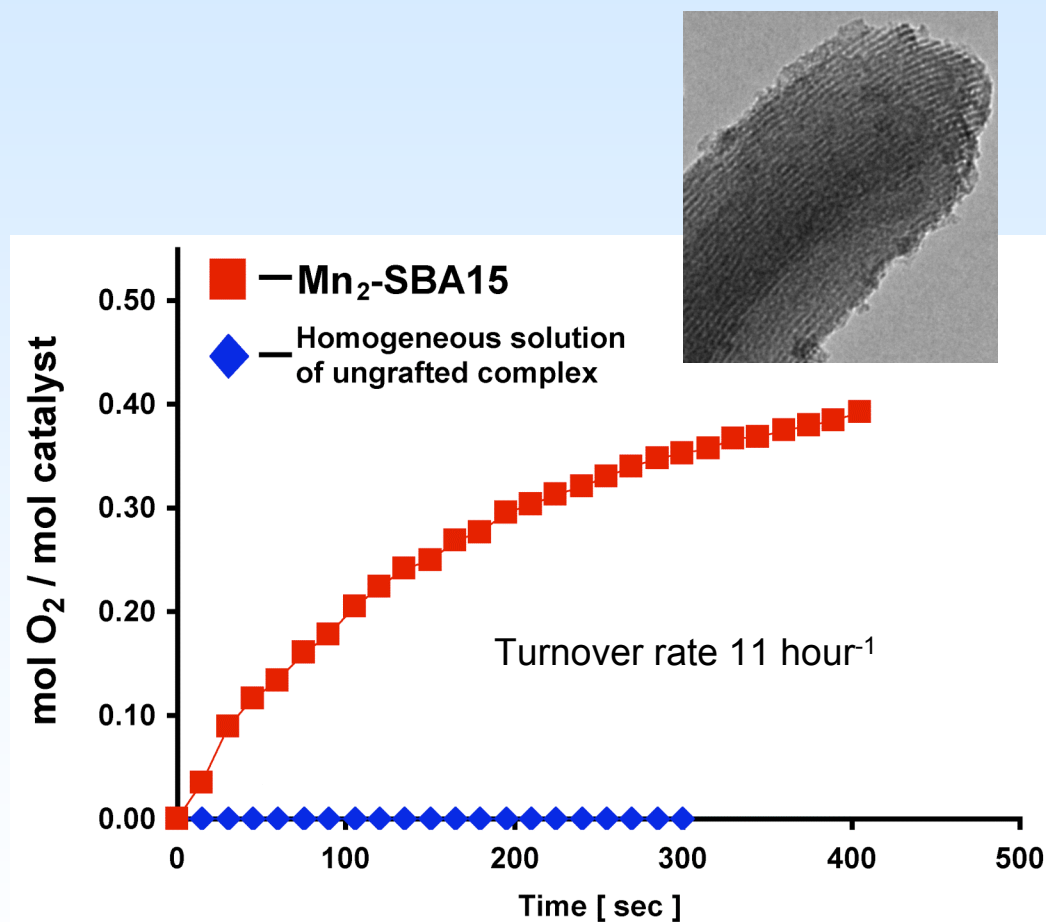
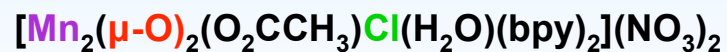
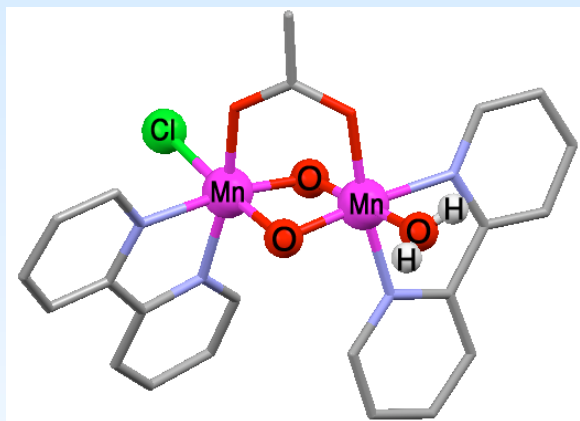


Turnover rate 300 s⁻¹



HELIOS

Synthetic Water Oxidation Catalyst on Nanoporous Silica Support

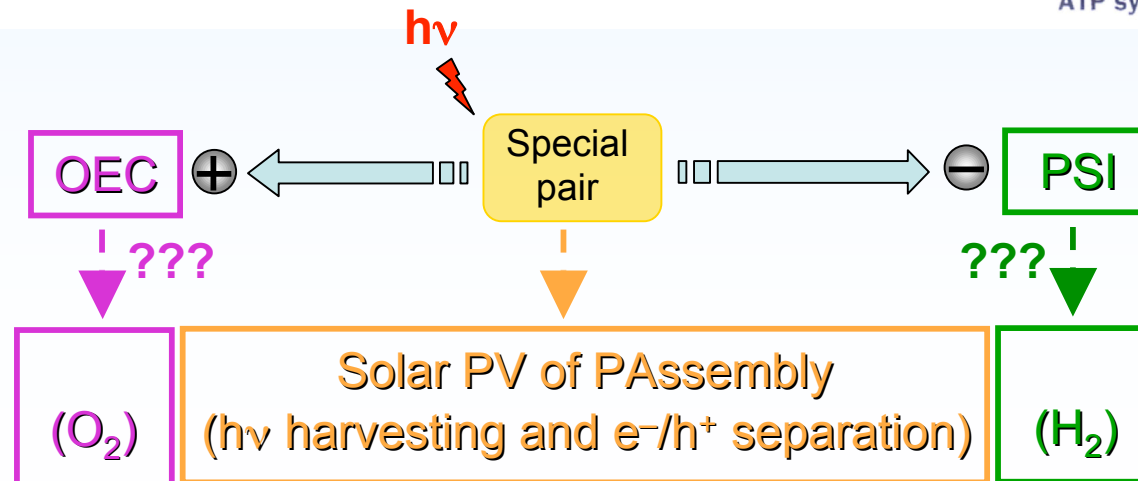
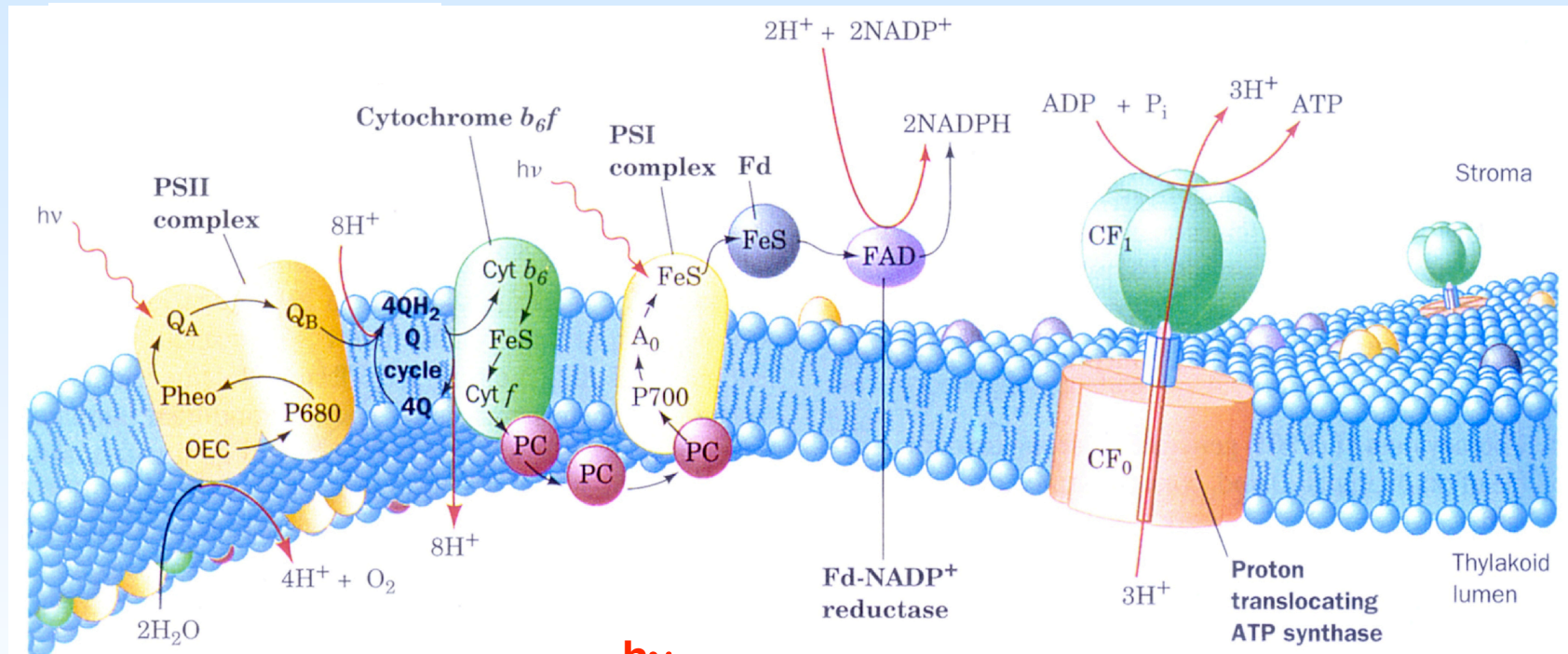


- O₂ evolution is only observed for Mn dimer complex in silica nanopores
- Turnover rate among the highest observed for synthetic Mn dimer catalyst



HELIOS

Photosynthetic membranes: natural vs. artificial



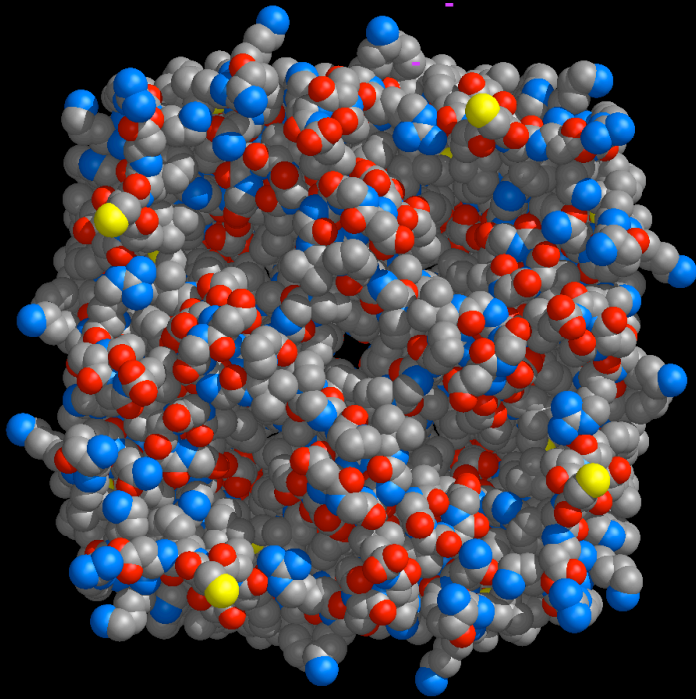


HELIOS



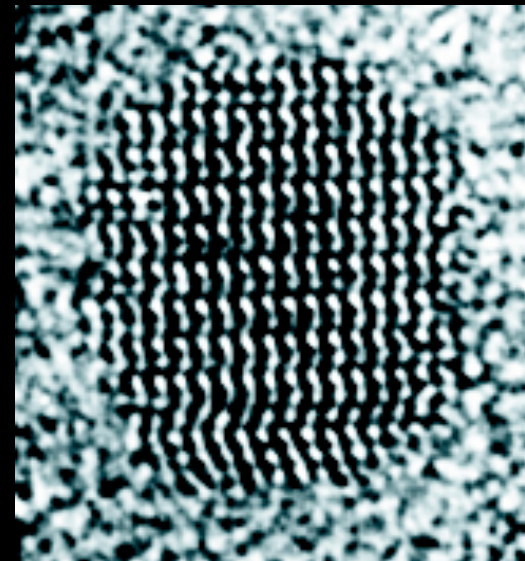
Conjunction of soft and hard matter

Protein



5nm

Nanocrystal



5nm



Helios Program in Solar Fuels Generation: complete the combustion cycle

